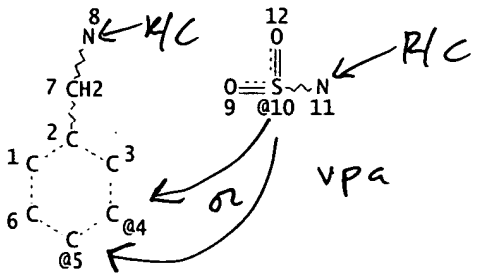
cpds related to CNS treatment

parent STR

```
=> d que l26
L1              STR
```

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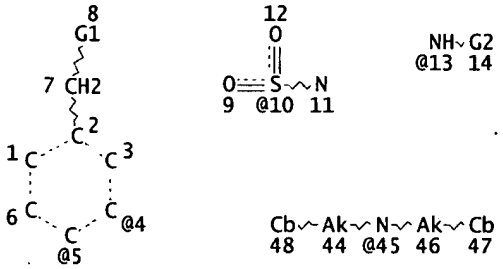
VPA 10-4/5 U
NODE ATTRIBUTES:
NSPEC   IS RC     AT   8
NSPEC   IS RC     AT  11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
L2          4364 SEA FILE=REGISTRY SSS FUL L1   4364 cpds
L8              STR      subset - fusion defining R1, R2
```

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@17  18  19       20 @21 22      24 @25 26      27 @28 29

 G3 N Ak         G4 N Ak Cb       Ak Cb        G5 N CH2 CH2 N
 30 @31 32       33 @34 35  36    @37 38       43 @42 41  40  39

VAR G1=45/25/21/13/23/28/31/34/42
VAR G2=15/16/17/37
VAR G3=16/37/17
VAR G4=15/16/17
VAR G5=15/16/37
VPA 10-4/5 U
NODE ATTRIBUTES:
NSPEC   IS RC     AT  11
NSPEC   IS RC     AT  19
NSPEC   IS R      AT  23
NSPEC   IS RC     AT  39
CONNECT IS E2  RC AT   1
CONNECT IS E2  RC AT   3
CONNECT IS E2  RC AT   6
CONNECT IS E1  RC AT  15
CONNECT IS E1  RC AT  20
CONNECT IS E1  RC AT  22
```

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CONNECT IS E1  RC AT  32
CONNECT IS E2  RC AT  35
CONNECT IS E2  RC AT  37
CONNECT IS E2  RC AT  44
CONNECT IS E2  RC AT  46
DEFAULT MLEVEL IS ATOM
GGCAT   IS SAT  AT  16
GGCAT   IS SAT  AT  24
GGCAT   IS SAT  AT  26
GGCAT   IS SAT  AT  29
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  48

STEREO ATTRIBUTES: NONE
L10        1458 SEA FILE=REGISTRY SUB=L2 SSS FUL L8   1458 cpds
L23         283 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L10
L24       24080 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CENTRAL NERVOUS/OBI
L25       10472 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CALCIUM CHANNEL/CT
L26           1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L23 AND (L24 OR L25)


=> d ibib abs hitstr l26

L26  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2003 ACS on STN          Applicant
ACCESSION NUMBER:         2001:50617  HCAPLUS
DOCUMENT NUMBER:          134:86033
TITLE:                    Preparation of sulfonamide substituted benzylamine
                          derivatives as calcium channels modulators
INVENTOR(S):              Milutinovic, Sandra Ginette; Simmonds, Robin George;
                          Tupper, David Edward
PATENT ASSIGNEE(S):       Eli Lilly and Company Limited, UK
SOURCE:                   PCT Int. Appl., 38 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
     WO 2001004087      A1   20010118       WO 2000-GB2361   20000615
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
             CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
             ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
             LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD,
             SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU,
             ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     GB 2352240         A1   20010124       GB 1999-16434    19990713
     EP 1200397         A1   20020502       EP 2000-938940   20000615
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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PRIORITY APPLN. INFO.:                    GB 1999-16434    A  19990713
                                          WO 2000-GB2361   W  20000615
OTHER SOURCE(S):          MARPAT 134:86033
GI
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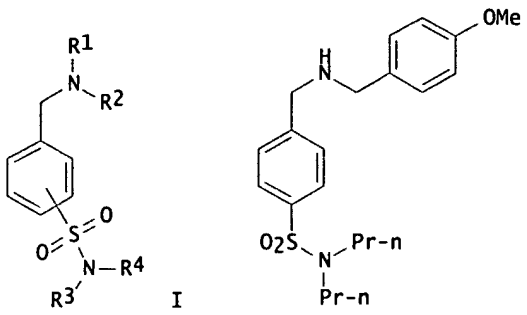


I II

AB The title compds. [I; the aminosulfonyl group is attached at the 3- or 4-position; R1 = H, alkyl, cycloalkyl, etc.; R2 = alkyl, cycloalkyl, cycloalkylalkyl, etc.; R3, R4 = alkyl, cycloalkyl, cycloalkylalkyl, etc.; or R1 and R2, or R3 and R4, together with the nitrogen atom to which they are attached, form (un)substituted carbocyclic group contg. 4-7 carbon atoms optionally contg. an oxygen atom or a further nitrogen atom, and said carbocyclic group being optionally fused to (un)substituted Ph] and their salts, useful in modulating the activity of calcium channels, were prepd. and formulated. E.g., a multi-step synthesis of benzenesulfonamide II as maleate salt was given. The exemplified compds. I are found to inhibit voltage-dependent calcium channels in cloned human cell lines expressing specific voltage-dependent calcium channels with an IC50 of < 10 .mu.M.

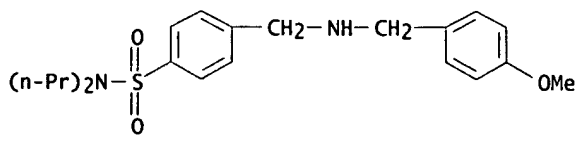
IT **317813-43-7P 317813-45-9P 317813-47-1P**
317813-49-3P 317813-51-7P 317813-53-9P
317813-55-1P 317813-57-3P 317813-59-5P
317813-61-9P 317813-63-1P 317813-65-3P
317813-66-4P 317813-68-6P 317813-70-0P
317813-72-2P 317813-74-4P 317813-76-6P
317813-77-7P 317813-80-2P 317813-81-3P
317813-83-5P 317813-84-6P 317813-85-7P
317813-86-8P 317813-87-9P 317813-88-0P
317813-89-1P 317813-91-5P 317813-92-6P
317813-93-7P 317813-94-8P 317813-95-9P
317813-96-0P 317813-97-1P 317813-98-2P
317814-02-1P 317814-04-3P 317814-05-4P
317814-06-5P 317814-07-6P 317814-08-7P
317814-09-8P 317814-10-1P 317814-11-2P
317814-13-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of sulfonamide substituted benzylamine derivs. as calcium channels modulators)

RN 317813-43-7 HCAPLUS

CN Benzenesulfonamide, 4-[[[(4-methoxyphenyl)methyl]amino]methyl]-N,N-dipropyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

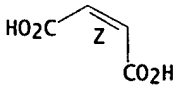
CRN 317813-42-6
CMF C21 H30 N2 O3 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

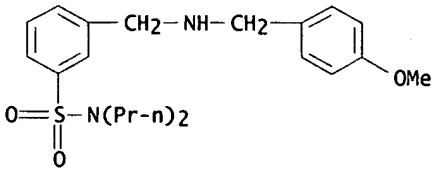
Double bond geometry as shown.



RN 317813-45-9 HCAPLUS
CN Benzenesulfonamide, 3-[[[(4-methoxyphenyl)methyl]amino]methyl]-N,N-dipropyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

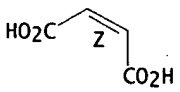
CRN 317813-44-8
CMF C21 H30 N2 O3 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

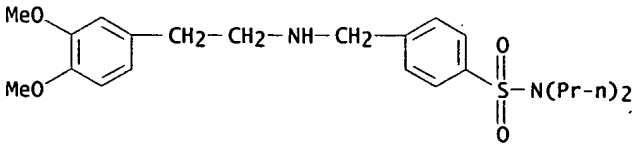
Double bond geometry as shown.



RN 317813-47-1 HCAPLUS
CN Benzenesulfonamide, 4-[[[2-(3,4-dimethoxyphenyl)ethyl]amino]methyl]-N,N-dipropyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

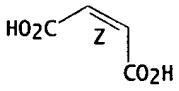
CRN 317813-46-0
CMF C23 H34 N2 O4 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

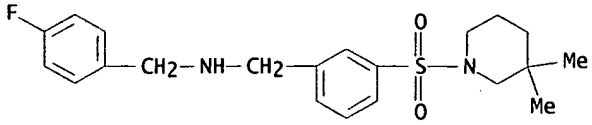
Double bond geometry as shown.



RN 317813-49-3 HCAPLUS
CN Piperidine, 1-[[3-[[[(4-fluorophenyl)methyl]amino]methyl]phenyl]sulfonyl]-3,3-dimethyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

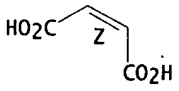
CRN 317813-48-2
CMF C21 H27 F N2 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

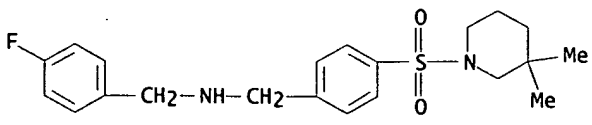
Double bond geometry as shown.



RN 317813-51-7 HCAPLUS
CN Piperidine, 1-[[4-[[[(4-fluorophenyl)methyl]amino]methyl]phenyl]sulfonyl]-3,3-dimethyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

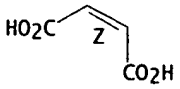
CRN 317813-50-6
CMF C21 H27 F N2 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

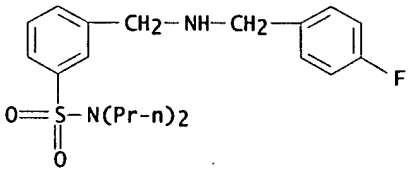
Double bond geometry as shown.



RN 317813-53-9 HCAPLUS
CN Benzenesulfonamide, 3-[[[(4-fluorophenyl)methyl]amino]methyl]-N,N-dipropyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

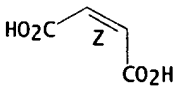
CRN 317813-52-8
CMF C20 H27 F N2 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

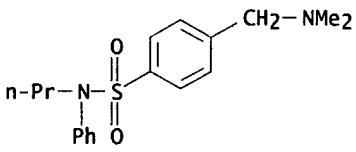
Double bond geometry as shown.



RN 317813-55-1 HCAPLUS
CN Benzenesulfonamide, 4-[(dimethylamino)methyl]-N-phenyl-N-propyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

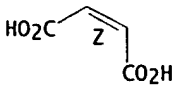
CRN 317813-54-0
CMF C18 H24 N2 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

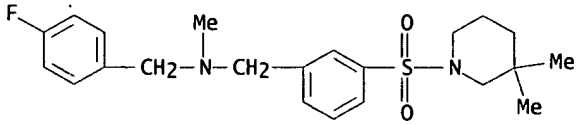
Double bond geometry as shown.



RN 317813-57-3 HCAPLUS
CN Piperidine, 1-[[3-[[[(4-fluorophenyl)methyl]methylamino]methyl]phenyl]sulfonyl]-3,3-dimethyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

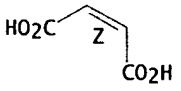
CRN 317813-56-2
CMF C22 H29 F N2 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

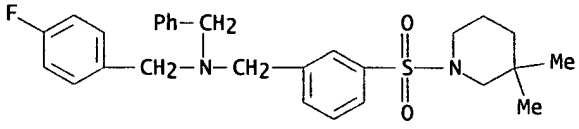
Double bond geometry as shown.



RN 317813-59-5 HCAPLUS
CN Piperidine, 1-[[3-[[[(4-fluorophenyl)methyl](phenylmethyl)amino]methyl]phenyl]sulfonyl]-3,3-dimethyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

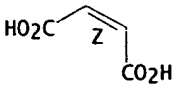
CRN 317813-58-4
CMF C28 H33 F N2 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

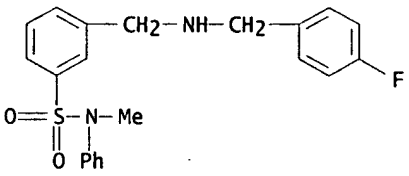
Double bond geometry as shown.



RN 317813-61-9 HCAPLUS
CN Benzenesulfonamide, 3-[[[(4-fluorophenyl)methyl]amino]methyl]-N-methyl-N-phenyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

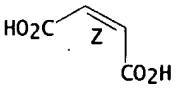
CRN 317813-60-8
CMF C21 H21 F N2 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

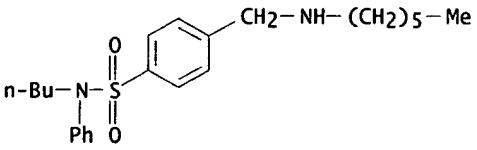
Double bond geometry as shown.



RN 317813-63-1 HCAPLUS
CN Benzenesulfonamide, N-butyl-4-[(hexylamino)methyl]-N-phenyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

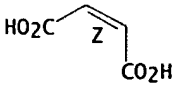
CRN 317813-62-0
CMF C23 H34 N2 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

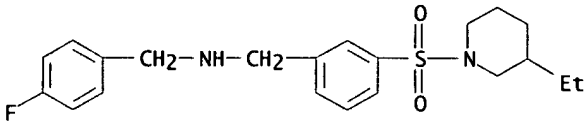
Double bond geometry as shown.



RN 317813-65-3 HCAPLUS
CN Piperidine, 3-ethyl-1-[[3-[[[(4-fluorophenyl)methyl]amino]methyl]phenyl]sulfonyl]-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

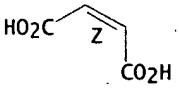
CRN 317813-64-2
CMF C21 H27 F N2 O2 S



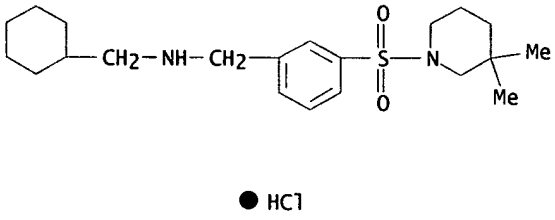
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 317813-66-4 HCAPLUS
CN Piperidine, 1-[[3-[[(cyclohexylmethyl)amino]methyl]phenyl]sulfonyl]-3,3-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)

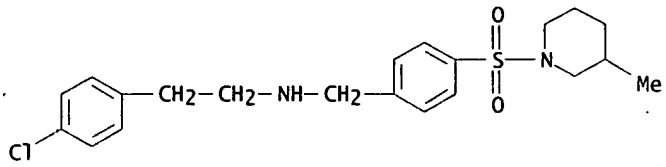


● HCl

RN 317813-68-6 HCAPLUS
CN Piperidine, 1-[[4-[[[2-(4-chlorophenyl)ethyl]amino]methyl]phenyl]sulfonyl]-3-methyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

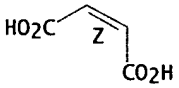
CRN 317813-67-5
CMF C21 H27 Cl N2 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

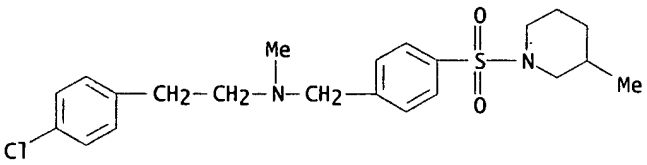
Double bond geometry as shown.



RN 317813-70-0 HCAPLUS
CN Piperidine, 1-[[4-[[[2-(4-chlorophenyl)ethyl]methylamino]methyl]phenyl]sulfonyl]-3-methyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

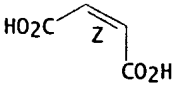
CRN 317813-69-7
CMF C22 H29 Cl N2 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

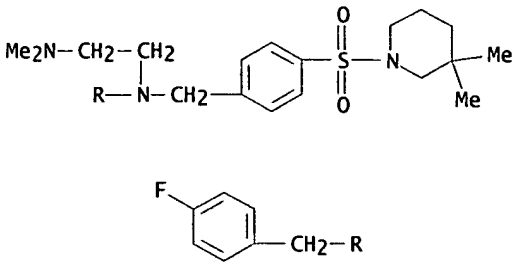
Double bond geometry as shown.



RN 317813-72-2 HCAPLUS
CN Piperidine, 1-[[4-[[[2-(dimethylamino)ethyl][(4-fluorophenyl)methyl]amino]methyl]phenyl]sulfonyl]-3,3-dimethyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

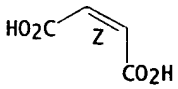
CRN 317813-71-1
CMF C25 H36 F N3 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

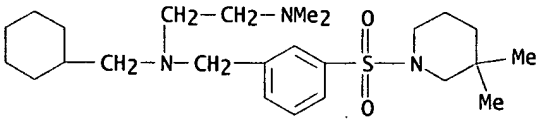
Double bond geometry as shown.



RN 317813-74-4 HCAPLUS
CN Piperidine, 1-[[3-[[(cyclohexylmethyl)[2-(dimethylamino)ethyl]amino]methyl]phenyl]sulfonyl]-3,3-dimethyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

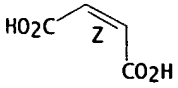
CRN 317813-73-3
CMF C25 H43 N3 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

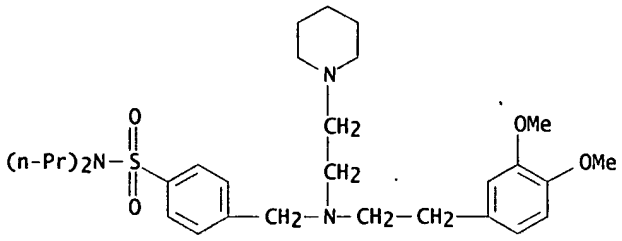


RN 317813-76-6 HCAPLUS
CN Benzenesulfonamide, 4-[[[2-(3,4-dimethoxyphenyl)ethyl][2-(1-piperidinyl)ethyl]amino]methyl]-N,N-dipropyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 317813-75-5

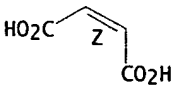
CMF C30 H47 N3 O4 S



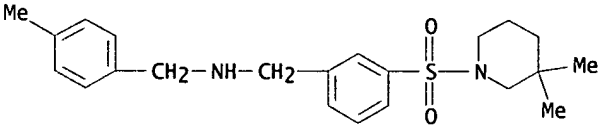
CM 2

CRN 110-16-7
CMF C4 H4 O4

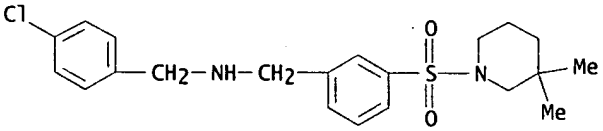
Double bond geometry as shown.



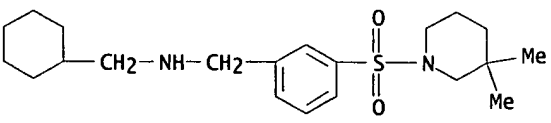
RN 317813-77-7 HCAPLUS
CN Piperidine, 3,3-dimethyl-1-[[3-[[[(4-methylphenyl)methyl]amino]methyl]phen
yl]sulfonyl]- (9CI) (CA INDEX NAME)



RN 317813-80-2 HCAPLUS
CN Piperidine, 1-[[3-[[[(4-chlorophenyl)methyl]amino]methyl]phenyl]sulfonyl]-
3,3-dimethyl- (9CI) (CA INDEX NAME)

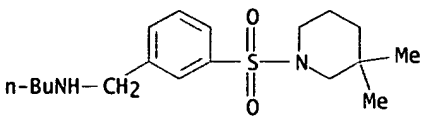


RN 317813-81-3 HCAPLUS
CN Piperidine, 1-[[3-[[(cyclohexylmethyl)amino]methyl]phenyl]sulfonyl]-3,3-
dimethyl- (9CI) (CA INDEX NAME)

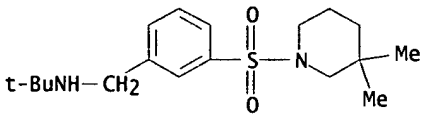


RN 317813-83-5 HCAPLUS
CN Piperidine, 1-[[3-[(butylamino)methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI)

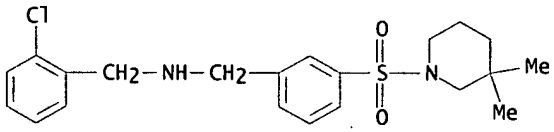
(CA INDEX NAME)



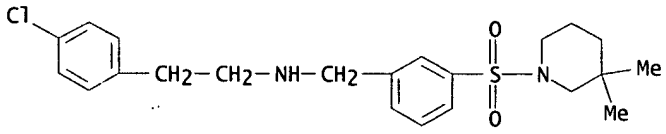
RN 317813-84-6 HCAPLUS
CN Piperidine, 1-[[3-[[(1,1-dimethylethyl)amino]methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)



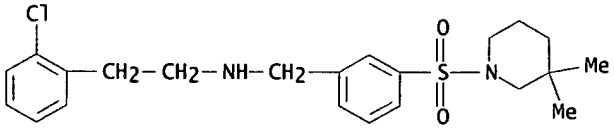
RN 317813-85-7 HCAPLUS
CN Piperidine, 1-[[3-[[[(2-chlorophenyl)methyl]amino]methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)



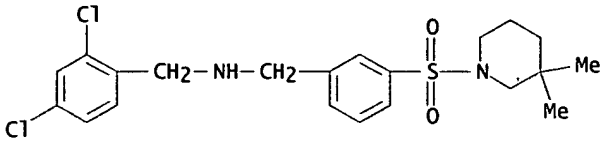
RN 317813-86-8 HCAPLUS
CN Piperidine, 1-[[3-[[[2-(4-chlorophenyl)ethyl]amino]methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)



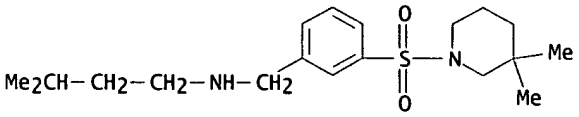
RN 317813-87-9 HCAPLUS
CN Piperidine, 1-[[3-[[[2-(2-chlorophenyl)ethyl]amino]methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)



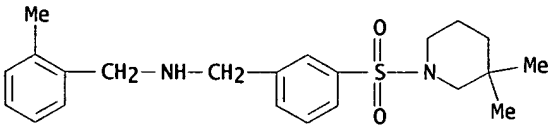
RN 317813-88-0 HCAPLUS
CN Piperidine, 1-[[3-[[[(2,4-dichlorophenyl)methyl]amino]methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)



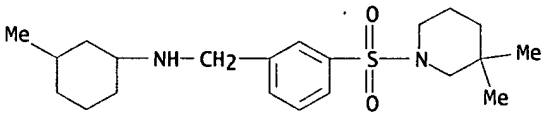
RN 317813-89-1 HCAPLUS
CN Piperidine, 3,3-dimethyl-1-[[3-[[(3-methylbutyl)amino]methyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



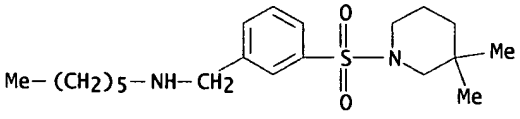
RN 317813-91-5 HCAPLUS
CN Piperidine, 3,3-dimethyl-1-[[3-[[[(2-methylphenyl)methyl]amino]methyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



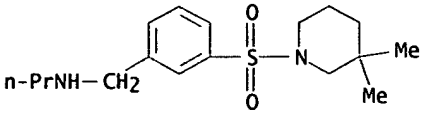
RN 317813-92-6 HCAPLUS
CN Piperidine, 3,3-dimethyl-1-[[3-[[(3-methylcyclohexyl)amino]methyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



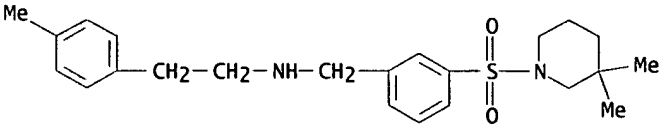
RN 317813-93-7 HCAPLUS
CN Piperidine, 1-[[3-[(hexylamino)methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)



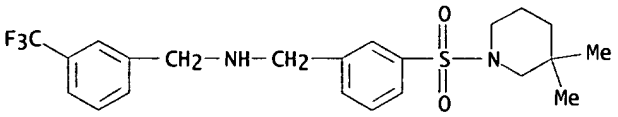
RN 317813-94-8 HCAPLUS
CN Piperidine, 3,3-dimethyl-1-[[3-[(propylamino)methyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



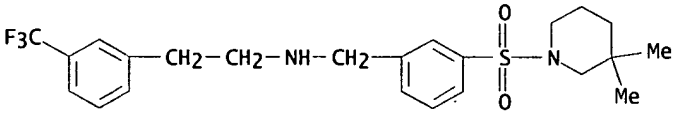
RN 317813-95-9 HCAPLUS
CN Piperidine, 3,3-dimethyl-1-[[3-[[[2-(4-methylphenyl)ethyl]amino]methyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



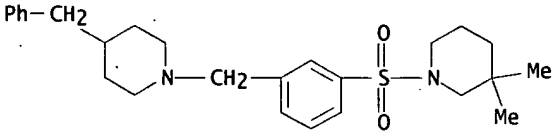
RN 317813-96-0 HCAPLUS
CN Piperidine, 3,3-dimethyl-1-[[3-[[[[3-(trifluoromethyl)phenyl]methyl]amino]methyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



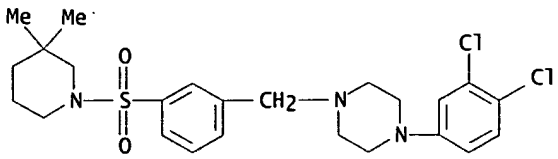
RN 317813-97-1 HCAPLUS
CN Piperidine, 3,3-dimethyl-1-[[3-[[[2-[3-(trifluoromethyl)phenyl]ethyl]amino]methyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



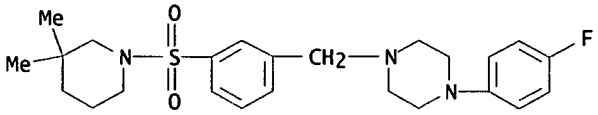
RN 317813-98-2 HCAPLUS
CN Piperidine, 3,3-dimethyl-1-[[3-[[4-(phenylmethyl)-1-piperidinyl]methyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



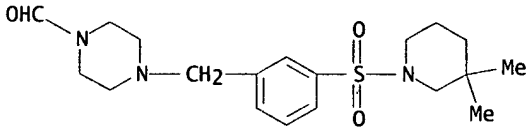
RN 317814-02-1 HCAPLUS
CN Piperidine, 1-[[3-[[4-(3,4-dichlorophenyl)-1-piperazinyl]methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)



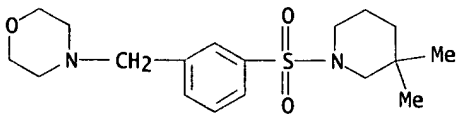
RN 317814-04-3 HCAPLUS
CN Piperidine, 1-[[3-[[4-(4-fluorophenyl)-1-piperazinyl]methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)



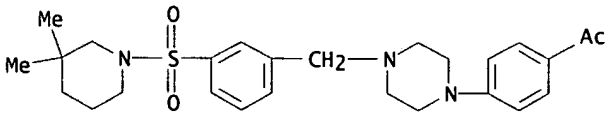
RN 317814-05-4 HCAPLUS
CN Piperidine, 1-[[3-[(4-formyl-1-piperazinyl)methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)



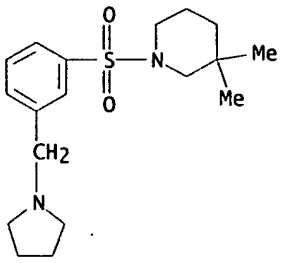
RN 317814-06-5 HCAPLUS
CN Piperidine, 3,3-dimethyl-1-[[3-(4-morpholinylmethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



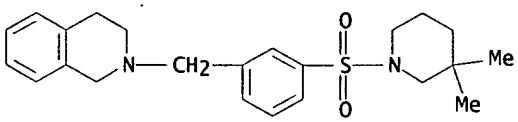
RN 317814-07-6 HCAPLUS
CN Piperidine, 1-[[3-[[4-(4-acetylphenyl)-1-piperazinyl]methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)



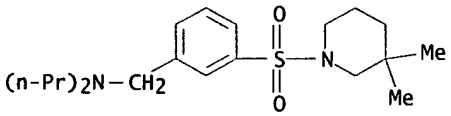
RN 317814-08-7 HCAPLUS
CN Piperidine, 3,3-dimethyl-1-[[3-(1-pyrrolidinylmethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



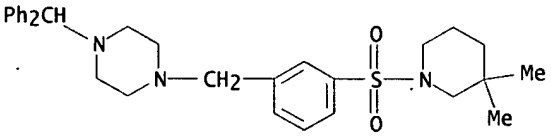
RN 317814-09-8 HCAPLUS
CN Piperidine, 1-[[3-[(3,4-dihydro-2(1H)-isoquinolinyl)methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)



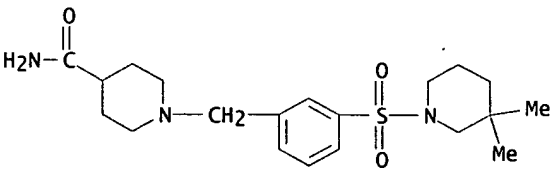
RN 317814-10-1 HCAPLUS
CN Piperidine, 1-[[3-[(dipropylamino)methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)



RN 317814-11-2 HCAPLUS
CN Piperidine, 1-[[3-[[4-(diphenylmethyl)-1-piperazinyl]methyl]phenyl]sulfonyl]-3,3-dimethyl- (9CI) (CA INDEX NAME)

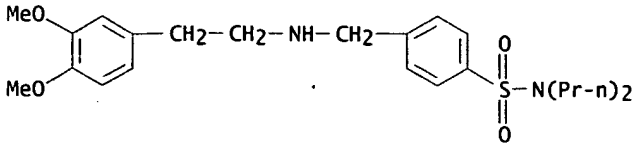


RN 317814-13-4 HCAPLUS
CN 4-Piperidinecarboxamide, 1-[[3-[(3,3-dimethyl-1-piperidinyl)sulfonyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



IT **317813-46-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of sulfonamide substituted benzylamine derivs. as calcium channels modulators)

RN 317813-46-0 HCAPLUS
CN Benzenesulfonamide, 4-[[[2-(3,4-dimethoxyphenyl)ethyl]amino]methyl]-N,N-dipropyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

compounds related to CCNS, nervous or neuron?)

KRISHNAN 10/031,122

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=> d que l28
L1              STR
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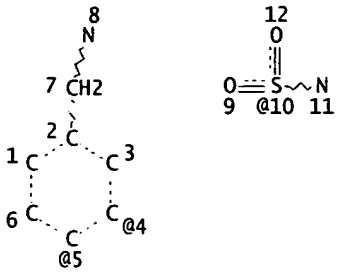


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NODE ATTRIBUTES:
NSPEC   IS RC     AT   8
NSPEC   IS RC     AT  11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
L2          4364 SEA FILE=REGISTRY SSS FUL L1
L8              STR
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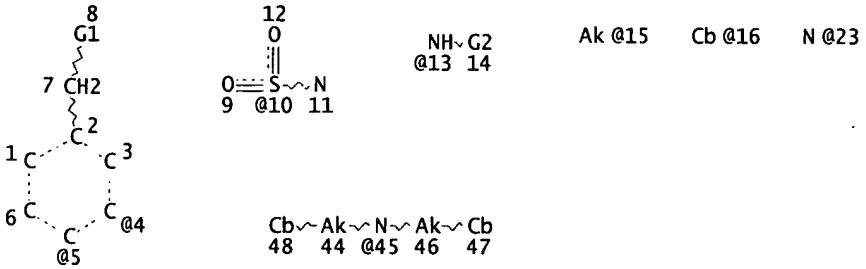


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VAR G2=15/16/17/37
VAR G3=16/37/17
VAR G4=15/16/17
VAR G5=15/16/37
VPA 10-4/5 U
NODE ATTRIBUTES:
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NSPEC   IS RC     AT  19
NSPEC   IS R      AT  23
NSPEC   IS RC     AT  39
CONNECT IS E2  RC AT   1
CONNECT IS E2  RC AT   3
CONNECT IS E2  RC AT   6
CONNECT IS E1  RC AT  15
CONNECT IS E1  RC AT  20
CONNECT IS E1  RC AT  22
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CONNECT IS E1  RC AT  32
CONNECT IS E2  RC AT  35
CONNECT IS E2  RC AT  37
CONNECT IS E2  RC AT  44
CONNECT IS E2  RC AT  46
DEFAULT MLEVEL IS ATOM
GGCAT   IS SAT  AT  16
GGCAT   IS SAT  AT  24
GGCAT   IS SAT  AT  26
GGCAT   IS SAT  AT  29
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  48

STEREO ATTRIBUTES: NONE
L10        1458 SEA FILE=REGISTRY SUB=L2 SSS FUL L8
L23         283 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L10
L27          14 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L23 AND  (NERVOUS OR NEURON?
                OR CNS)
L28           8 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L27 AND PY<2001


=> d ibib abs hitstr 1

L28  ANSWER 1 OF 8  HCAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         2000:707143  HCAPLUS
DOCUMENT NUMBER:          133:266722
TITLE:                    Preparation of 1-arenesulfonyl-2-aryl-pyrrolidine and
                          piperidine derivatives as metabotropic glutamate
                          receptor antagonists/agonists for the treatment of
                          CNS disorders
INVENTOR(S):              Mutel, Vincent; Vieira, Eric; Wichmann, Jurgen
PATENT ASSIGNEE(S):       F. Hoffmann-La Roche A.-G., Switz.
SOURCE:                   PCT Int. Appl., 42 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
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     WO 2000058285      A1   20001005       WO 2000-EP2431   20000318 <--
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             JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG,
             MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,
             TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ,
             MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     NZ 514037          A    20010928       NZ 2000-514037   20000318
     BR 2000009278      A    20011226       BR 2000-9278     20000318
     EP 1165510         A1   20020102       EP 2000-910863   20000318
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     US 6284785         B1   20010904       US 2000-534380   20000324
     HR 2001000682      A1   20021031       HR 2001-682      20010917
     ZA 2001007689      A    20021218       ZA 2001-7689     20010918
     NO 2001004617      A    20010924       NO 2001-4617     20010924
PRIORITY APPLN. INFO.:                    EP 1999-106004   A  19990325
                                          WO 2000-EP2431   W  20000318
OTHER SOURCE(S):          MARPAT 133:266722
GI
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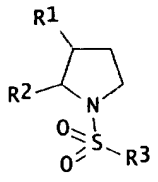

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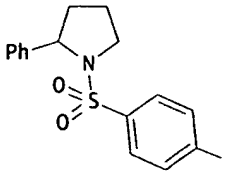


II

AB The title compds. I [R1 = H, alkyl, hydroxyalkyl; R2 = furyl, thienyl, pyridyl or Ph {optional substituents selected from alkyl, alkoxy, halogen, cyano, CF3, amine, dialkylamine}; R3 = naphthyl or Ph {optional substituents selected from alkyl, alkoxy, halogen, acetyl, cyano, hydroxyalkyl, -CH2-morpholin-4-yl, alkyloxyalkyl, alkyl-N(R4)2 or CF3}; R4 = H, alkyl], as well as their pharmaceutically acceptable salts, were prepd. for the treatment of CNS disorders. For example, compd. II was prepd. by sulfonation of 2-phenylpyrrolidine with p-toluenesulfonyl chloride. II demonstrated agonistic behavior (IC50 = 0.23.mu.M) toward metabotropic glutamate receptor.

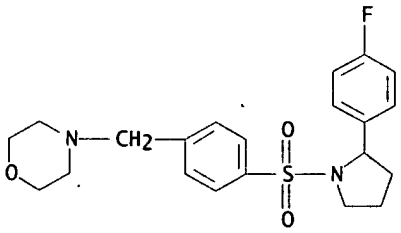
IT **298690-64-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compds.; prepn. of arenesulfonylaryl-pyrrolidine and -piperidine derivs. as metabotropic glutamate receptor antagonists/agonists)

RN 298690-64-9 HCAPLUS

CN Pyrrolidine, 2-(4-fluorophenyl)-1-[[4-(4-morpholinylmethyl)phenyl]sulfonyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

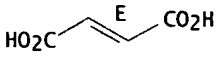
CRN 298690-63-8
CMF C21 H25 F N2 O3 S



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

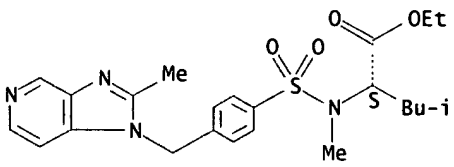
=> d ibib abs hitstr 2

L28 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:506576 HCAPLUS
DOCUMENT NUMBER: 131:153649
TITLE: Randomized trial of the platelet-activating factor antagonist lexipafant in HIV-associated cognitive impairment
AUTHOR(S): Schifitto, G.; Sacktor, N.; Marder, K.; McDermott, M. P.; McArthur, J. C.; Kieburtz, K.; Small, S.; Epstein, L. G.
CORPORATE SOURCE: University of Rochester Medical Center, Rochester, NY, USA
SOURCE: Neurology (1999), 53(2), 391-396
CODEN: NEURAI; ISSN: 0028-3878
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The aim of this study was to assess the safety and tolerability of lexipafant in HIV-assocd. cognitive impairment. Cognitive impairment is the most common neurol. complication of advanced HIV-1 infection. There is evidence that a variety of inflammatory mediators, including platelet-activating factor (PAF), may contribute to **neuronal** injury. We hypothesized that lexipafant, a PAF antagonist, might improve cognitive dysfunction in HIV-infected people. We conducted a randomized, double-blind, placebo-controlled clin. trial to assess the safety and tolerability of lexipafant 500 mg/day. The primary outcome measure for tolerability was the ability to complete the study on the originally assigned dosage of medication. Thirty patients with cognitive impairment were enrolled. Lexipafant was safe and well tolerated. Ninety-three percent in the placebo group and 88% in the lexipafant group completed the study at the originally assigned dosage. Trends toward improvement were seen in neuropsychol. performance, esp. verbal memory, in the lexipafant treatment group. This study shows that lexipafant, the first PAF antagonist used in HIV-assocd. cognitive impairment, is a safe and well tolerated compd. The obsd. trends toward improvement in neuropsychol. test scores warrant the pursuit of a larger and longer efficacy trial to assess the impact of lexipafant on cognitive performance.

IT **139133-26-9**, Lexipafant
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effect of platelet-activating factor antagonist lexipafant in HIV-assocd. cognitive impairment)
RN 139133-26-9 HCAPLUS
CN L-Leucine, N-methyl-N-[[4-[(2-methyl-1H-imidazo[4,5-c]pyridin-1-yl)methyl]phenyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L28 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:805716 HCAPLUS
DOCUMENT NUMBER: 128:61509
TITLE: Preparation of aryl-substituted cyclic amines as

selective dopamine D3 ligands

INVENTOR(S): Haadsma-Svensson, Susanne R.; Cleek, Kerry Anne; Lin, Chiu-Hong; Leiby, Jeffrey A.; Darlington, William H.; Romero, Arthur G.; et al.

PATENT ASSIGNEE(S): Pharmacia & Upjohn Company, USA; Haadsma-Svensson, Susanne R.; Cleek, Kerry Anne; Lin, Chiu-Hong; Leiby, Jeffrey A.; Darlington, William H.; Romero, Arthur G.

SOURCE: PCT Int. Appl., 73 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9745403	A1	19971204	WO 1997-US7650	19970512 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9730601	A1	19980105	AU 1997-30601	19970512 <--
AU 720414	B2	20000601		
CN 1217711	A	19990526	CN 1997-194326	19970512 <--
EP 923542	A1	19990623	EP 1997-925470	19970512 <--
EP 923542	B1	20030820		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2000511529	T2	20000905	JP 1997-542424	19970512 <--
NZ 332538	A	20010223	NZ 1997-332538	19970512
RU 2185372	C2	20020720	RU 1998-123954	19970512
SK 282725	B6	20021106	SK 1998-1488	19970512
AT 247639	E	20030915	AT 1997-925470	19970512
US 6084130	A	20000704	US 1997-859587	19970520 <--
FI 9802572	A	19981127	FI 1998-2572	19981127 <--
KR 2000016147	A	20000325	KR 1998-709715	19981128 <--
NO 9805599	A	19981130	NO 1998-5599	19981130 <--

PRIORITY APPLN. INFO.: US 1996-18794P P 19960531
WO 1997-US7650 W 19970512

OTHER SOURCE(S): MARPAT 128:61509

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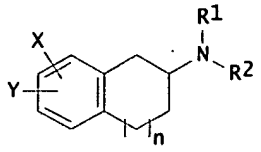

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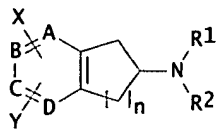

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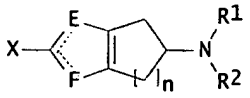

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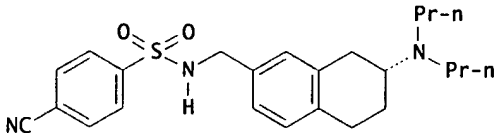


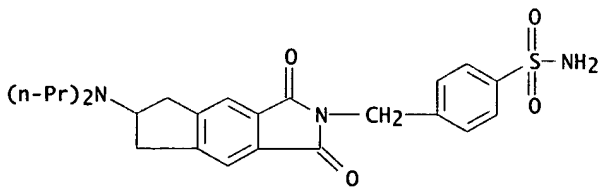
IV

AB The title compds. [I (wherein X, Y are at the 5-7 position; when n = 1 then X = (CH2)mCONR4R5, (CH2)mSO2R3, etc.; m = 0-1; Y = R4, halo, etc.; when n = 0 or 1 then XY = C(O)NR10C(O), CH2NR10C(O), etc.; when n = 0 and Y = OR9 then X = (CH2)mCONR4R5, (CH2)mSO2NR4R5, etc.; R1, R2 = H, C1-8 alkyl, C1-8 alkylaryl; R3 = C1-8 alkyl, C1-6 alkylaryl, aryl; R4, R5 = H, C1-8 alkyl, C1-6 alkylaryl, aryl; R9 = C2-8 alkyl, C1-6 alkylaryl, aryl; R10 = H, C1-8 alkyl, etc.), II (wherein one of A-D is N and the remaining positions are CH; n = 1-2; X = (CH2)mCONR4R5, (CH2)mSO2R3, etc.; m = 0-1; Y = R4, halo, etc.; XY = C(O)NR4C(O), CH2NR4C(O), etc.; R1-R5 as above), III (one of E or F is N and the other is S; n= 1-2; X, R1-R5 as above)], useful for treating central nervous system disorders assocd. with dopamine D3 receptor activity, were prepd.. Thus, reaction of (R)-7-(dipropylamino)-5,6,7,8-tetrahydro-2-naphthalenemethanamine with 4-cyanophenylsulfonyl chloride afforded (+)-(R)-IV which showed Ki of 32 nM against D3 receptor binding vs. Ki of 1436 nM against D2 receptor binding.

IT **200187-22-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of aryl-substituted cyclic amines as selective dopamine D3 ligands)

RN 200187-22-0 HCAPLUS

CN Benzenesulfonamide, 4-[[6-(dipropylamino)-3,5,6,7-tetrahydro-1,3-dioxocyclopent[f]isoindol-2(1H)-yl]methyl]- (9CI) (CA INDEX NAME)



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L28 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

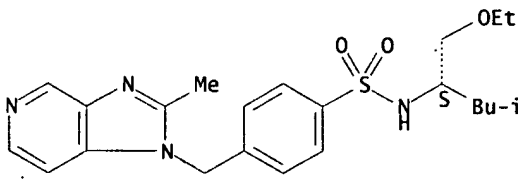
ACCESSION NUMBER: 1997:710904 HCAPLUS
DOCUMENT NUMBER: 127:355275
TITLE: Effects of combined glutamate and platelet-activating factor inhibition on the outcome of focal cerebral ischemia - an initial screening study
AUTHOR(S): Aspey, B. S.; Alp, M. S.; Patel, Y.; Harrison, M. J. G.
CORPORATE SOURCE: Reta Lila Weston Institute of Neurological Studies, UCL Medical School, London, W1P 6DB, UK
SOURCE: Metabolic Brain Disease (1997), 12(3), 237-249
CODEN: MBDIEE; ISSN: 0885-7490
PUBLISHER: Plenum
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Since both glutamate excitotoxicity and inflammatory responses have been implicated in ischemic **neuronal** death, we questioned whether joint inhibition of both processes would be more neuroprotective than either on its own. Therefore we assessed the effects of combined inhibition of both glutamate release (with a use-dependant sodium channel blocker, 619C89) and inflammatory processes (with a platelet-activating factor (PAF) receptor antagonist, BB-823) on the degree of motor deficit and the extent of cerebral (cortical and sub-cortical gray matter) infarction produced by middle cerebral artery occlusion (MCAO) in the rat, and compared results to appropriate single agent, vehicle and pos. controls. The combination of both agents produced the greatest redn. in motor deficit, but the effect was only significant ($p<0.05$) acutely (4 to 6 h post-MCAO). The extent of cortical infarction at 24 h post-MCAO was significantly reduced in all exptl. groups compared to vehicle-controls ($p<0.05$) and the greatest redn. occurred in the combination group (55%), though it was not significantly better than either of the single agent groups. Similarly the greatest redn. in sub-cortical infarction was in the combination group, but this was also not significantly better than the single agents. The results of this novel combination of pharmacol. interventions suggest that inhibition of both glutamate excitotoxicity and inflammatory responses afforded an overall enhanced, if modest, neuroprotective effect, compared to inhibition of either process alone. The possible mechanisms involved are discussed, but warrant further clarification before therapeutic strategies are developed.

IT **139133-28-1**, BB-823
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(combined glutamate and platelet-activating factor inhibition effect on cerebral ischemia outcome)

RN 139133-28-1 HCAPLUS
CN Benzenesulfonamide, N-[(1S)-1-(ethoxymethyl)-3-methylbutyl]-4-[(2-methyl-1H-imidazo[4,5-c]pyridin-1-yl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L28 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:694212 HCAPLUS
DOCUMENT NUMBER: 125:328730

TITLE: Preparation of 3-(piperazinoalkyl)indole derivatives as calmodulin antagonists
INVENTOR(S): Hasegawa, Atsushi; Makino, Tooru; Yamamoto, Kenjiro
PATENT ASSIGNEE(S): Daiichi Seiyaku Co, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 49 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08225535	A2	19960903	JP 1995-294071	19951113 <--

PRIORITY APPLN. INFO.: JP 1994-280963 19941115
OTHER SOURCE(S): MARPAT 125:328730
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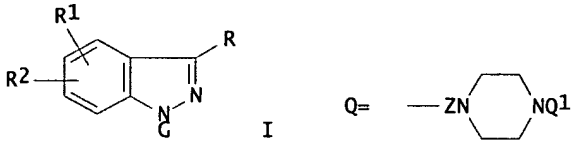

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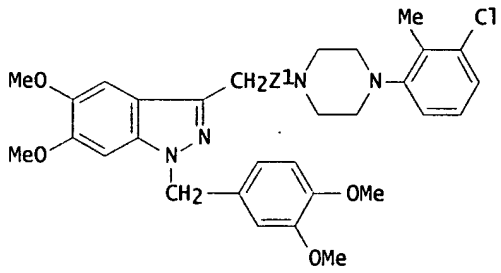


II

AB The title compds. [I; R = Q; wherein Z = single bond, C1-3 alkylene, C2-4 alkenylene, C1-3 hydroxyalkylene, CO, COCO, C1-2 alkylene contg. one CO group at the end or middle of the C chain; Q1 = C1-8 alkyl, C3-8 cycloalkyl, (un)substituted aryl, heterocyclyl, diarylmethyl, or aryl-C1-6 alkyl; R1, R2 = C1-6 alkyl or alkoxy, CF3, CF3CH2, CF3O, CF3CH2O, C1-6 alkylthio, alkylsulfinyl, or alkylsulfonyl, C1-6 alkylcarbonyl, C2-7 alkanoylamino, NH2, mono- di(C1-6 alkyl)amino, OH, halo, C2-6 perfluoroalkyl, cyano, NO2, CO2H, C1-6 alkoxycarbonyl, tetrazolyl, SO2NH2, methylenedioxy, ethylenedioxy, morpholinosulfonyl, piperazinosulfonyl, 4-(C1-6 alkyl)piperazinosulfonyl, 4-[mono- or di(C1-6 alkyl)amino]piperidino, 4-aminopiperidino; G = C1-6 alkyl, (un)substituted Ph, PhCO, PhCOCH2, .alpha.-hydroxybenzyl, phenyl-C1-6 alkyl, 5-membered arom. heterocyclyl or heterocyclyl-C1-6 alkyl contg. heteroatoms (a) N, O, or S or (b) one or two N and another N, O, or S, 6-membered arom. heterocyclyl, heterocyclylcarbonyl, or heterocyclyl-C1-3 alkyl contg. one or two N, phenylhydroxyalkyl, or 2-phenylethynyl, tetrazolyl, morpholino, etc.] are prepd. These compds. possess calmodulin-inhibitory, antihypoxic, or brain edema-improving activity, inhibit delayed neuronal death in hippocampus, and are useful for the treatment of circulatory diseases or brain diseases. Thus, 5,6-dimethoxy-1-(3,4-dimethoxybenzyl)-1H-indazole-3-acetic acid was condensed with 1-(3-chloro-2-methylphenyl)piperazine using di(2-pyridyl) disulfide and Ph3P in CH2Cl2 at room temp. to give an intermediate (II; Z1 = CO), which was reduced by borane-THF complex in THF under reflux to give the title compd. II (Z1 = CH2). The latter compd. in vitro showed IC50 of 3.1 .mu.g/mL against Ca/calmodulin-dependent phosphodiesterase.

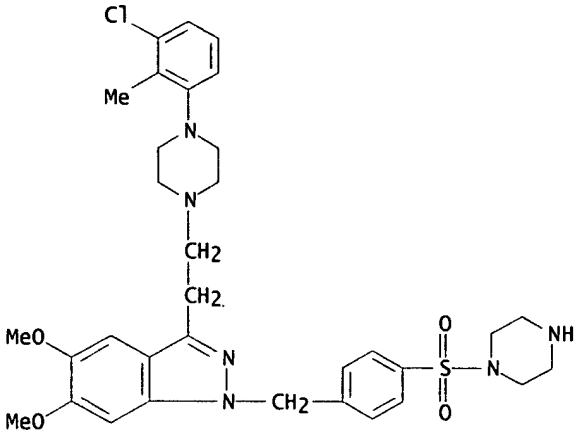
IT **183315-54-0P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-(piperazinoalkyl)indole derivs. as calmodulin antagonists for disease treatment)

RN 183315-54-0 HCAPLUS

CN Piperazine, 1-[[4-[[3-[2-[4-(3-chloro-2-methylphenyl)-1-piperazinyl]ethyl]-5,6-dimethoxy-1H-indazol-1-yl]methyl]phenyl]sulfonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

●2 HCl

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L28 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:401562 HCAPLUS
DOCUMENT NUMBER: 125:86674
TITLE: (Azetidin-1-ylalkyl)lactams as tachykinin antagonists.
INVENTOR(S): Mackenzie, Alexander Roderick; Marchington, Alan Patrick; Middleton, Donald Stuart; Meadows, Sandra Dora
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Research and Development Company, N.V./s.A.; Pfizer Inc.
SOURCE: PCT Int. Appl., 286 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9605193	A1	19960222	WO 1995-EP3054	19950729 <--
W: AU, CA, CN, CZ, FI, HU, JP, KR, MX, NO, NZ, PL, RU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
TW 432061	B	20010501	TW 1995-84107375	19950717
CA 2197086	AA	19960222	CA 1995-2197086	19950729 <--
AU 9532549	A1	19960307	AU 1995-32549	19950729 <--
AU 689303	B2	19980326		
EP 775132	A1	19970528	EP 1995-929036	19950729 <--

EP 775132	B1	20010328			
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CN 1154699	A	19970716	CN 1995-194416	19950729	<--
CN 1072666	B	20011010			
JP 09508646	T2	19970902	JP 1995-506974	19950729	<--
HU 77771	A2	19980828	HU 1997-373	19950729	<--
RU 2150468	C1	20000610	RU 1997-104032	19950729	<--
AT 200083	E	20010415	AT 1995-929036	19950729	
JP 3159389	B2	20010423	JP 1996-506974	19950729	
ES 2155894	T3	20010601	ES 1995-929036	19950729	
PL 183180	B1	20020531	PL 1995-318534	19950729	
CZ 291544	B6	20030416	CZ 1997-381	19950729	
IL 114826	A1	19991231	IL 1995-114826	19950803	<--
BR 9503582	A	19960430	BR 1995-3582	19950808	<--
FI 9700523	A	19970207	FI 1997-523	19970207	<--
NO 9700566	A	19970207	NO 1997-566	19970207	<--
US 5968923	A	19991019	US 1997-798534	19970210	<--

PRIORITY APPLN. INFO.:

GB 1994-16084	A	19940809
GB 1994-17898	A	19940906
WO 1995-EP3054	W	19950729

OTHER SOURCE(S): MARPAT 125:86674

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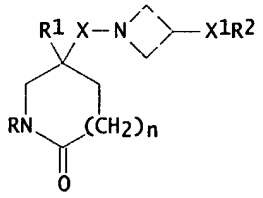

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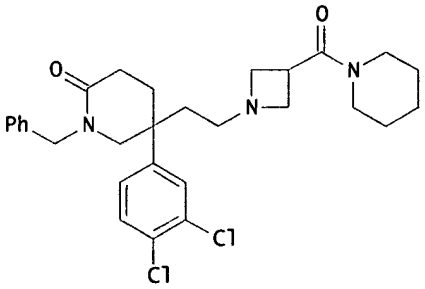


II

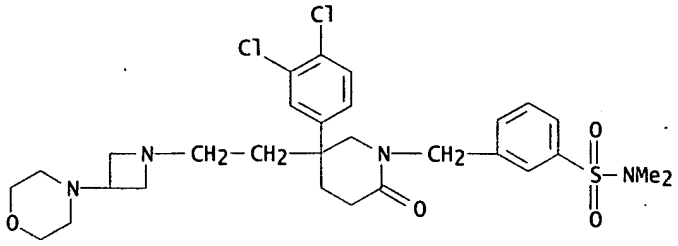
AB The invention provides compds. I and their pharmaceutically acceptable salts [wherein R = (un)substituted cycloalkyl, aryl, or alkyl; R1 = (un)substituted Ph, naphthyl, thienyl, benzothienyl, or indolyl; R2 = CO2H, (un)substituted CONH2, NH2, SO2NH2, etc., or various (un)substituted N-heterocyclic groups; X = C1-4 alkylene; X1 = bond or C1-6 alkylene; m = 0-2], together with preparative intermediates, compns. contg. the compds., and their use. as tachykinin antagonists. For example, reductive N-alkylation of 3-(1-piperidinocarbonyl)azetidine with the corresponding aldehyde [prepns. given] using NaBH(OAc)3 and AcOH in THF gave title compd. II. In a test for displacement of [125I]-NKA from cloned human NK2 receptors in vitro, II had pIC50 of 9.0. Examples include syntheses of approx. 120 I and approx. 190 intermediates, plus data for 6 compds. in 2 bioassays.

IT **178310-09-3P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of (azetidinylalkyl) lactams as tachykinin antagonists)

RN 178310-09-3 HCAPLUS
CN Benzenesulfonamide, 3-[[5-(3,4-dichlorophenyl)-5-[2-[3-(4-morpholinyl)-1-azetidinyl]ethyl]-2-oxo-1-piperidinyl]methyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



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L28 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:259446 HCAPLUS
DOCUMENT NUMBER: 124:289534
TITLE: 1-Benzyl-1,3-dihydro-2H-benzimidazol-2-one derivatives, their preparation, and pharmaceutical compositions containing them as vasopressin and/or oxytocin receptor ligands.
INVENTOR(S): Di Malta, Alain; Mettefeu, Daniel; Garcia, Georges; Roux, Richard; Serradeil-Legal, Claudine
PATENT ASSIGNEE(S): Sanofi, Fr.
SOURCE: Eur. Pat. Appl., 49 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 694536	A1	19960131	EP 1995-401599	19950704 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
FR 2722190	A1	19960112	FR 1994-8278	19940705 <--
FR 2722190	B1	19961004		
JP 08073439	A2	19960319	JP 1995-170048	19950705 <--
US 5661169	A	19970826	US 1995-498542	19950705 <--

PRIORITY APPLN. INFO.: FR 1994-8278 19940705
OTHER SOURCE(S): MARPAT 124:289534
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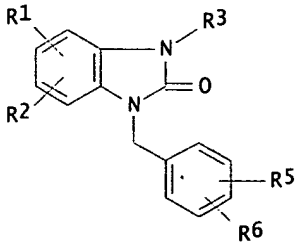

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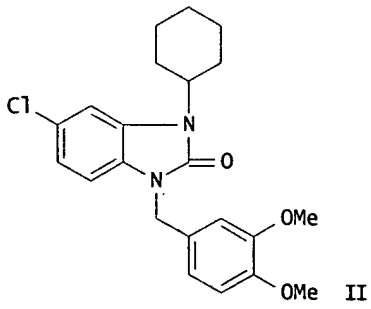


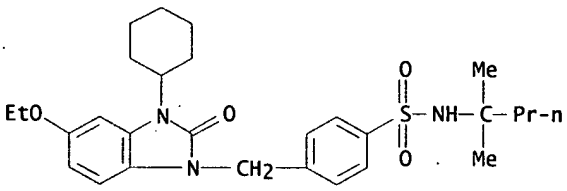
II

AB Over 50 examples of title compds. I [R1 = halo, alkyl, alkylthio, PhS, CF3, cyano, NO2, (un)substituted amino, OH, alkoxy, etc.; R2 = H, halo, alkyl; R3 = R4, (CH2)pR4, indanyl, adamantyl, (un)substituted cyclohexyl, etc.; R4 = (un)substituted amino, (un)substituted cycloalkyl, furyl, thienyl, pyrrolyl, pyridyl, etc.; R5 = H, alkyl, alkoxy, halo, OH, CF3; R6 = cyano, (un)substituted amino or aminomethyl, aryl, OH, alkoxy, etc.; p = 1-8] were prepd. For example, 2,4-dichloro-1-nitrobenzene underwent a sequence of condensation with cyclohexylamine, redn. of the nitro group, and cyclocondensation with urea, to give 5-chloro-3-cyclohexyl-1,3-dihydro-2H-benzimidazol-2-one. This was N-alkylated with 1-(bromomethyl)-3,4-dimethoxybenzene, using NaH in THF, to give title compd. II. In various receptor binding assays, I had IC50 values down to 10-6 M for V1, 10-9 M for V2, and 10-6 M for oxytocin receptors.

IT **175866-21-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzyldihydrobenzimidazolone derivs. as vasopressin and/or oxytocin receptor ligands)

RN 175866-21-4 HCAPLUS

CN Benzenesulfonamide, 4-[(3-cyclohexyl-5-ethoxy-2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)methyl]-N-(1,1-dimethylbutyl)- (9CI) (CA INDEX NAME)



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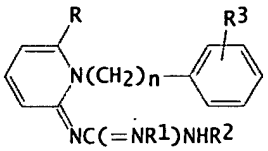
L28 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1976:135484 HCAPLUS
DOCUMENT NUMBER: 84:135484
TITLE: Pyridinylidene guanidines
INVENTOR(S): Yale, Harry L.; Bristol, James A.
PATENT ASSIGNEE(S): Squibb, E. R., and Sons, Inc., USA
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3933836	A	19760120	US 1974-509513	19740926 <--
CA 1054603	A1	19790515	CA 1975-234881	19750905 <--
FR 2285879	A1	19760423	FR 1975-29439	19750925 <--
FR 2285879	B1	19800530		
DE 2543031	A1	19760415	DE 1975-2543031	19750926 <--
JP 51059870	A2	19760525	JP 1975-117075	19750926 <--

PRIORITY APPLN. INFO.: US 1974-509513 19740926
GI



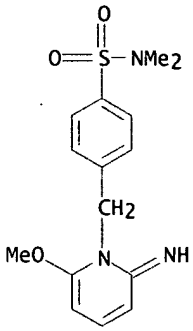
I

AB Five guanidines I (R = H, OMe; R1, R2 = Me2CH, cyclohexyl, Ph; R3 = H, 2-Br, 4-Me2NSO2; n = 1 or 2), useful as central **nervous** system stimulants (dosages given but not activity), were prepd. by reaction of pyridinimines with carbodiimides. Thus, 2-aminopyridine was quaternized with PhCH2Br to 2-amino-1-(phenylmethyl)pyridinium bromide, which was heated with MeONa in MeOH at reflux, and the resulting pyridinimine treated with dicyclohexylcarbodiimide in Me3COH at reflux to give I (R = R3 = H; R1 = R2 = cyclohexyl; n = 1).

IT **58804-21-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with cyclohexylphenylcarbodiimide)

RN 58804-21-0 HCAPLUS

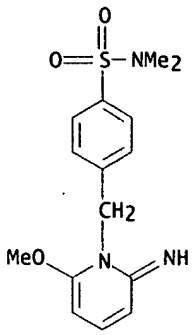
CN Benzenesulfonamide, 4-[(2-imino-6-methoxy-1(2H)-pyridinyl)methyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



IT **58804-20-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with sodium methoxide)

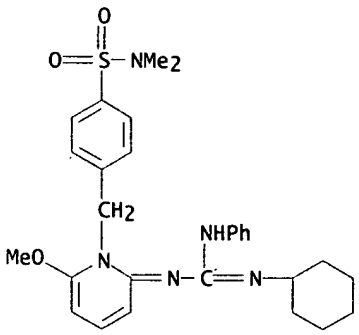
RN 58804-20-9 HCAPLUS

CN Benzenesulfonamide, 4-[(2-imino-6-methoxy-1(2H)-pyridinyl)methyl]-N,N-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT **58804-22-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 58804-22-1 HCAPLUS
CN Benzenesulfonamide, 4-[[2-[[(cyclohexylamino)(phenylimino)methyl]imino]-6-methoxy-1(2H)-pyridinyl]methyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



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L28 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:707143 HCAPLUS
DOCUMENT NUMBER: 133:266722
TITLE: Preparation of 1-arenesulfonyl-2-aryl-pyrrolidine and piperidine derivatives as metabotropic glutamate receptor antagonists/agonists for the treatment of CNS disorders
INVENTOR(S): Mutel, Vincent; Vieira, Eric; Wichmann, Jurgen
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000058285	A1	20001005	WO 2000-EP2431	20000318 <--
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
NZ 514037	A	20010928	NZ 2000-514037	20000318
BR 2000009278	A	20011226	BR 2000-9278	20000318
EP 1165510	A1	20020102	EP 2000-910863	20000318
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6284785	B1	20010904	US 2000-534380	20000324
HR 2001000682	A1	20021031	HR 2001-682	20010917
ZA 2001007689	A	20021218	ZA 2001-7689	20010918
NO 2001004617	A	20010924	NO 2001-4617	20010924

PRIORITY APPLN. INFO.: EP 1999-106004 A 19990325
WO 2000-EP2431 W 20000318

OTHER SOURCE(S): MARPAT 133:266722
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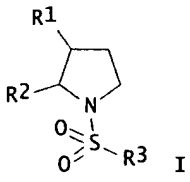

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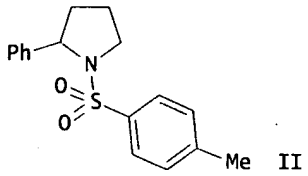

II

AB The title compds. I [R1 = H, alkyl, hydroxyalkyl; R2 = furyl, thienyl, pyridyl or Ph {optional substituents selected from alkyl, alkoxy, halogen, cyano, CF3, amine, dialkylamine}; R3 = naphthyl or Ph {optional substituents selected from alkyl, alkoxy, halogen, acetyl, cyano, hydroxyalkyl, -CH2-morpholin-4-yl, alkyloxyalkyl, alkyl-N(R4)2 or CF3}; R4 = H, alkyl], as well as their pharmaceutically acceptable salts, were prepd. for the treatment of CNS disorders. For example, compd. II was prepd. by sulfonation of 2-phenylpyrrolidine with p-toluenesulfonyl chloride. II demonstrated agonistic behavior (IC50 = 0.23.mu.M) toward metabotropic glutamate receptor.

IT **298690-64-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compds.; prepn. of arenesulfonylaryl-pyrrolidine and -piperidine derivs. as metabotropic glutamate receptor antagonists/agonists)

RN 298690-64-9 HCAPLUS
CN Pyrrolidine, 2-(4-fluorophenyl)-1-[[4-(4-morpholinylmethyl)phenyl]sulfonyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

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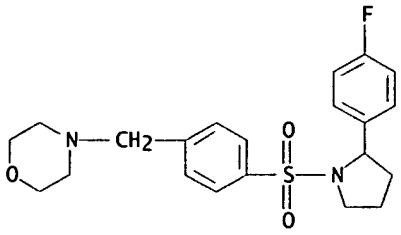
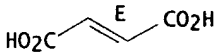
CRN 298690-63-8
CMF C21 H25 F N2 O3 S



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



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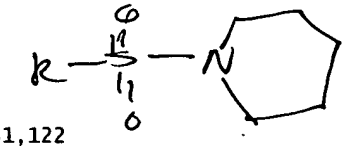
cpds having 

KRISHNAN 10/031,122

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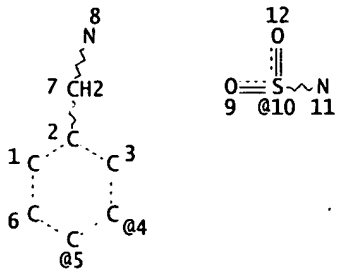

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 12

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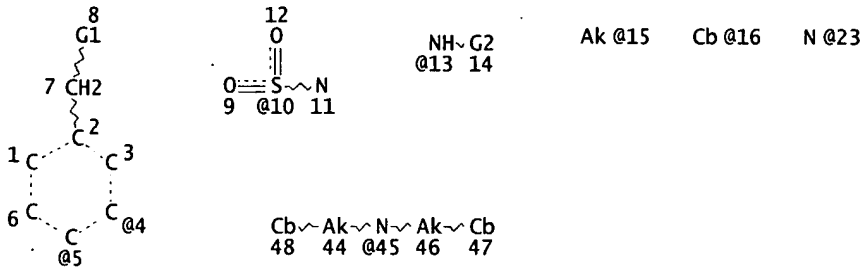

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Ak~Cb
@37 38

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GRAPH ATTRIBUTES:
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L25       10472 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CALCIUM CHANNEL/CT
L26           1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L23 AND (L24 OR L25)
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L37           7 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L36 NOT L26


=> d ibib abs hitstr 1

L37  ANSWER 1 OF 7  HCAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:        1999:511143  HCAPLUS
DOCUMENT NUMBER:         131:170361
TITLE:                   Preparation of sulfonamides as inhibitors of activated
                         blood coagulation factor X
INVENTOR(S):             Tawada, Hiroyuki; Itoh, Fumio; Banno, Hiroshi;
                         Terashita, Zenichi
PATENT ASSIGNEE(S):      Takeda Chemical Industries, Ltd., Japan
SOURCE:                  PCT Int. Appl., 187 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                Japanese
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.       KIND  DATE           APPLICATION NO.  DATE
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     WO 9940075        A1   19990812       WO 1999-JP470    19990204 <--
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             MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM,
             TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
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     AU 9922988        A1   19990823       AU 1999-22988    19990204 <--
     JP 2000204081     A2   20000725       JP 1999-27053    19990204 <--
     EP 1054005        A1   20001122       EP 1999-902829   19990204 <--
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             IE, FI
     US 6403595        B1   20020611       US 2000-601660   20000803
     US 2002193382     A1   20021219       US 2002-128809   20020424
PRIORITY APPLN. INFO.:                   JP 1998-24833    A  19980205
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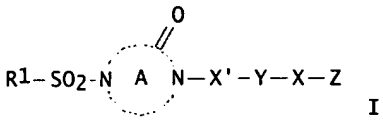
JP 1998-317205 A 19981109
WO 1999-JP470 W 19990204
US 2000-601660 A3 20000803

OTHER SOURCE(S): MARPAT 131:170361

GI



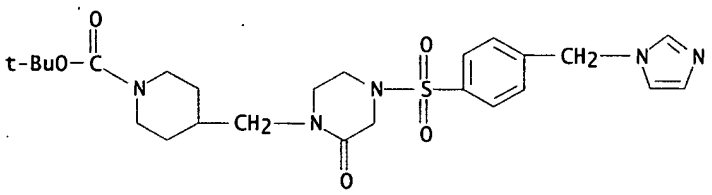
I

AB The title compds. I [R1 represents a hydrocarbyl or heterocyclic group each optionally substituted; the ring A represents a divalent nitrogen-contg. heterocycle group optionally further substituted; X' represents optionally substituted alkylene; Y represents an optionally substituted divalent cyclic group; X represents a bond or optionally substituted alkylene; and Z represents optionally substituted amino, optionally substituted imidoyl, or an optionally substituted nitrogen-contg. heterocyclic group] are prepd. Formulations contg. a compd. of this invention are given. In a test for inhibiting activity of title compds. against activated blood coagulation factor X, 1-(4-amidinobenzyl)-4-(6-chloronaphthalene-2-sulfonyl)-2-piperazinone hydrochloride showed IC50 of 0.05 .mu.M.

IT **239073-24-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of sulfonamides as inhibitors of activated blood coagulation factor X)

RN 239073-24-6 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[[4-(1H-imidazol-1-ylmethyl)phenyl]sulfonyl]-2-oxo-1-piperazinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 2

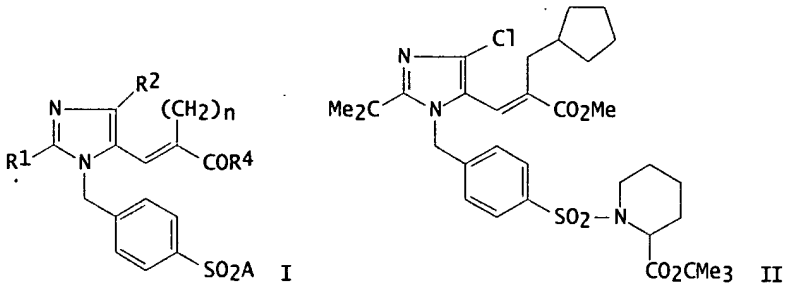
L37 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:217671 HCAPLUS
DOCUMENT NUMBER: 120:217671
TITLE: Sulfonylbenzyl substituted imidazolylpropenic acid derivatives
INVENTOR(S): Hanko, Rudolf; Dressel, Juergen; Fey, Peter; Huebsch, Walter; Kraemer, Thomas; Mueller, Ulrich; Mueller-Gliemann, Matthias; Beuck, Margin; Kazda, Stanislav; et al.
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Eur. Pat. Appl., 37 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
EP 557842	A2	19930901	EP 1993-102322	19930215	<--
EP 557842	A3	19940406			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE					
DE 4206041	A1	19930902	DE 1992-4206041	19920227	<--
US 5475016	A	19951212	US 1993-19001	19930218	<--
CA 2090281	AA	19930828	CA 1993-2090281	19930224	<--
AU 9333769	A1	19930902	AU 1993-33769	19930224	<--
JP 06116244	A2	19940426	JP 1993-58057	19930224	<--
ZA 9301367	A	19931011	ZA 1993-1367	19930226	<--
HU 64056	A2	19931129	HU 1993-544	19930226	<--
CN 1075963	A	19930908	CN 1993-101882	19930227	<--
US 5627285	A	19970506	US 1995-524279	19950906	<--

PRIORITY APPLN. INFO.: DE 1992-4206041 19920227
US 1993-19001 19930218

OTHER SOURCE(S): CASREACT 120:217671; MARPAT 120:217671
GI

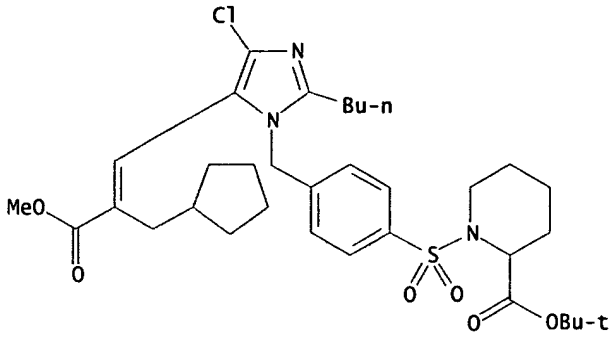


AB The title compds., 2-alkyl-3-[1-(4-sulfonylbenzyl)-1H-imidazolyl]propenoates I (R1 = alkyl, cycloalkyl, etc.; R2 = hydrogen, halo, etc.; R3 = hydrogen, alkyl, etc.; R4 = hydroxy, alkoxy, amino; A = tetrazolyl, heteroaryl, etc.) and their uses as pharmaceuticals are claimed. More specifically, I are antihypertensives, i.e. I have activity as angiotensin II antagonists, and I are agents for the treatment of atherosclerosis. Some I were tested for natriuretic activity in rats. An example compd., (.+-.)-3-[1-[4-[[2-(tert-butylalkoxycarbonyl)-1-piperidinyl]sulfonyl]benzyl]-4-chloro-2-isopropyl-5-imidazolyl]propenoate II was prepd. in several steps.

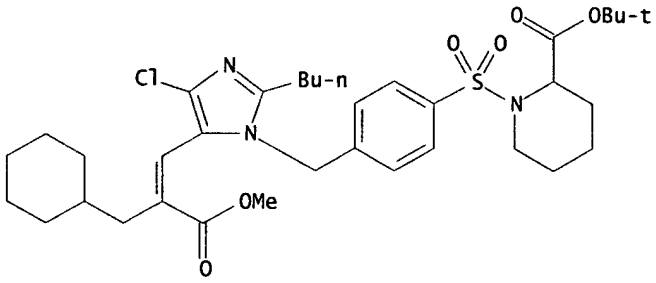
IT **153250-78-3P 153250-79-4P 153250-93-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as antiatherosclerotic and antihypertensive)

RN 153250-78-3 HCAPLUS

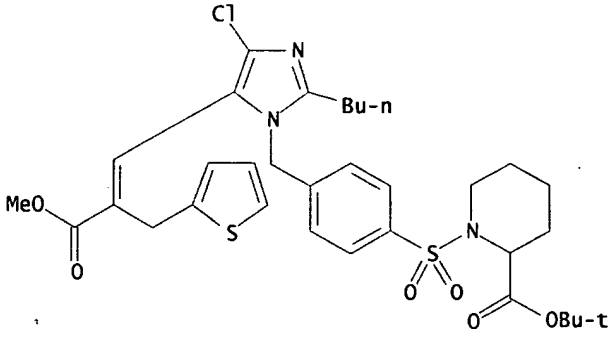
CN 2-Piperidinecarboxylic acid, 1-[[4-[[2-butyl-4-chloro-5-[2-(cyclopentylmethyl)-3-methoxy-3-oxo-1-propenyl]-1H-imidazol-1-yl]methyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



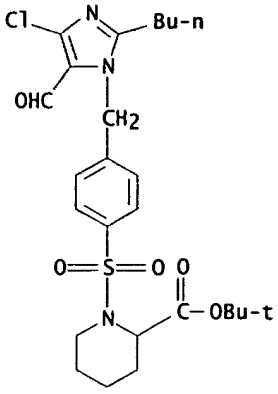
RN 153250-79-4 HCAPLUS
CN 2-Piperidinecarboxylic acid, 1-[[4-[[2-butyl-4-chloro-5-[2-(cyclohexylmethyl)-3-methoxy-3-oxo-1-propenyl]-1H-imidazol-1-yl]methyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 153250-93-2 HCAPLUS
CN 2-Piperidinecarboxylic acid, 1-[[4-[[2-butyl-4-chloro-5-[3-methoxy-3-oxo-2-(2-thienylmethyl)-1-propenyl]-1H-imidazol-1-yl]methyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



IT **152297-04-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for alkyl[(sulfonylbenzyl)imidazolyl]propenoate (antihypertensive and antiatherosclerotic))
RN 152297-04-6 HCAPLUS
CN 2-Piperidinecarboxylic acid, 1-[[4-[(2-butyl-4-chloro-5-formyl-1H-imidazol-1-yl)methyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

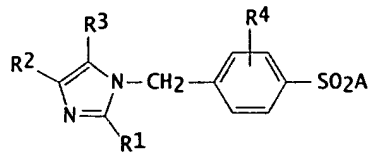


=> d ibib abs hitstr 3

L37 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:107008 HCAPLUS
DOCUMENT NUMBER: 120:107008
TITLE: Preparation of sulfonylbenzylimidazoles as angiotensin II antagonists
INVENTOR(S): Hanko, Rudolf; Dressel, Juergen; Fey, Peter; Huebsch, Walter; Kraemer, Thomas; Mueller, Ulrich; Mueller-Gliemann, Matthias; Beuck, Martin; Kazda, Stanislav; et al.
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 19 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4206043	A1	19930902	DE 1992-4206043	19920227 <--
EP 562261	A2	19930929	EP 1993-102324	19930215 <--
EP 562261	A3	19940413		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
US 5318980	A	19940607	US 1993-18961	19930218 <--
CA 2090274	AA	19930828	CA 1993-2090274	19930224 <--
AU 9333771	A1	19930902	AU 1993-33771	19930224 <--
ZA 9301369	A	19930924	ZA 1993-1369	19930226 <--
HU 64332	A2	19931228	HU 1993-540	19930226 <--
JP 06041087	A2	19940215	JP 1993-61347	19930226 <--
CN 1077710	A	19931027	CN 1993-102461	19930227 <--

PRIORITY APPLN. INFO.: DE 1992-4206043 19920227
OTHER SOURCE(S): MARPAT 120:107008
GI



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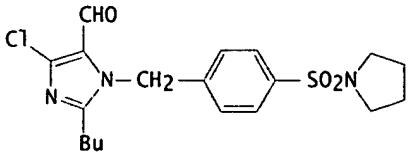


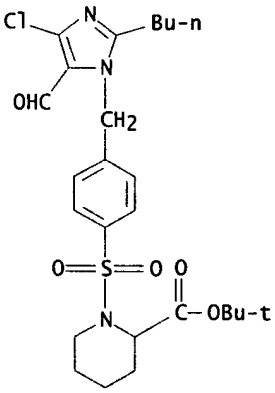
II

AB Title compds. [I; R1 = (cycloalkyl-substituted) alkyl, alkenyl; R2 = H, halo, perfluoroalkyl; R3 = (HO- or alkoxy-substituted) alkyl, COR5, CONR5R6; R5 = H, alkoxy, OH, PhO; R6, R7 = H, alkyl, Ph; R4 = H, halo, perfluoroalkyl; A = (substituted) 3-8 membered satd. heterocyclyl], were prepd. Thus, 2-butyl-4-chloro-5-formylimidazole was stirred with NaH in DMF; 4-bromomethyl benzenesulfonyl pyrrolidinide (prepn. given) in DMF was added and the mixt. was stirred 2.5 h to give title compd. II. Compd. I inhibited angiotensin II - induced contraction of guinea pig aortal rings with IC50 = 15-16 nM.

IT **152297-04-6P 152297-07-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as angiotensin II antagonist)

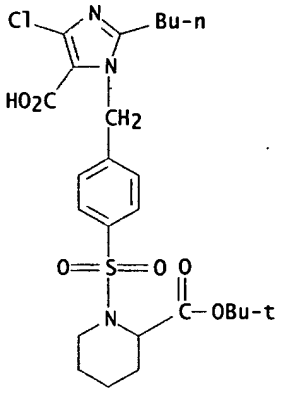
RN 152297-04-6 HCAPLUS

CN 2-Piperidinecarboxylic acid, 1-[[4-[(2-butyl-4-chloro-5-formyl-1H-imidazol-1-yl)methyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 152297-07-9 HCAPLUS

CN 2-Piperidinecarboxylic acid, 1-[[4-[(2-butyl-5-carboxy-4-chloro-1H-imidazol-1-yl)methyl]phenyl]sulfonyl]-, 2-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

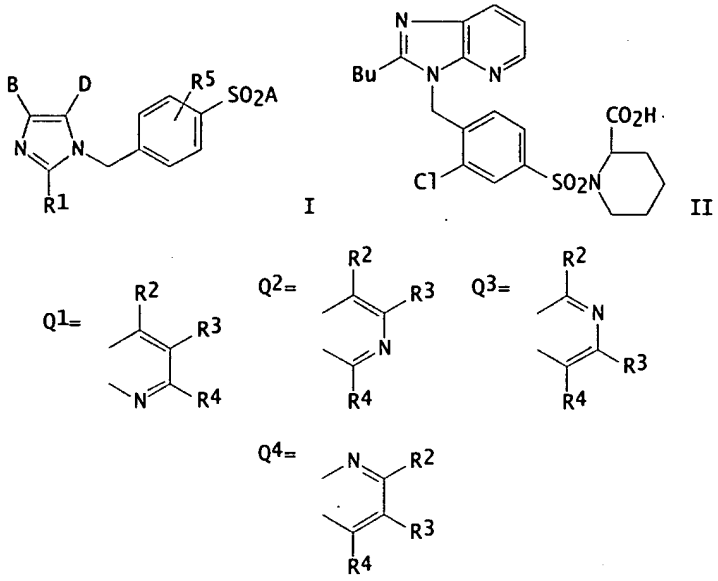


=> d ibib abs hitstr 4

L37 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:107007 HCAPLUS
DOCUMENT NUMBER: 120:107007
TITLE: Preparation of sulfonylbenzyl-substituted imidazopyridines as angiotensin II antagonists
INVENTOR(S): Hanko, Rudolf; Dressel, Juergen; Fey, Peter; Huebsch, Walter; Kraemer, Thomas; Mueller, Ulrich; Mueller-Gliemann, Matthias; Beuck, Martin; Kazda, Stanislav; et al.
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 20 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4206042	A1	19930902	DE 1992-4206042	19920227 <--
EP 564788	A2	19931013	EP 1993-102325	19930215 <--
EP 564788	A3	19931020		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
US 5364942	A	19941115	US 1993-18964	19930218 <--
CA 2090279	AA	19930828	CA 1993-2090279	19930224 <--
AU 9333772	A1	19930902	AU 1993-33772	19930224 <--
JP 06049068	A2	19940222	JP 1993-61077	19930225 <--
HU 64341	A2	19931228	HU 1993-543	19930226 <--
CN 1077195	A	19931013	CN 1993-102154	19930227 <--

PRIORITY APPLN. INFO.: DE 1992-4206042 19920227
OTHER SOURCE(S): MARPAT 120:107007
GI

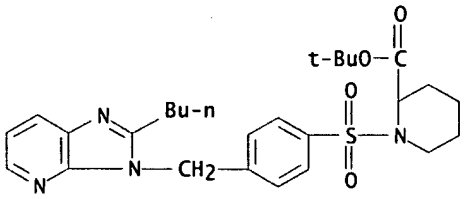


AB Title compds. [I; R1 = cycloalkyl, (cycloalkyl-substituted) alkyl, alkenyl; BD = Q1-Q4; R2, R3 = H, halo, alkyl; R4 = R2, COR6; R6 = OH, alkoxy, PhO, amino; R5 = H, halo, alkyl, perfluoroalkyl; A = (substituted) 3-8 membered heterocyclyl], were prepd. Thus, 4-bromomethyl-3-chlorobenzenesulfonyl N-2-(tert-butoxycarbonyl)piperidinide (prepn. given) was stirred with 2-butylimidazo[4,5-b]pyridine and NaH in DMF to give 30% coupling product, which was treated with CF3CO2H to give 99% title compd. II. I inhibited angiotensin II-induced contraction of guinea pig aorta rings with IC50 = 40-326 nM. I also inhibited proliferation of rat and swine smooth muscle cells in vitro.

IT **152531-06-1P 152531-12-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as angiotensin II antagonist)

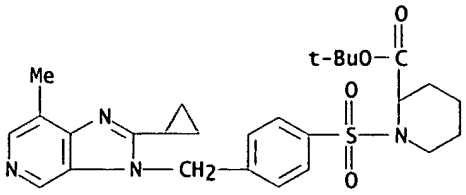
RN 152531-06-1 HCAPLUS

CN 2-Piperidinecarboxylic acid, 1-[[4-[(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)methyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 152531-12-9 HCAPLUS

CN 2-Piperidinecarboxylic acid, 1-[[4-[(2-cyclopropyl-7-methyl-3H-imidazo[4,5-c]pyridin-3-yl)methyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



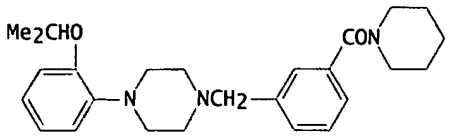
=> d ibib abs hitstr 5

L37 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1993:517276 HCAPLUS
DOCUMENT NUMBER: 119:117276
TITLE: Novel 4-arylpiperazines and 4-arylpiperidines
INVENTOR(S): Reitz, Allen B.
PATENT ASSIGNEE(S): McNeilab, Inc., USA
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9304682	A1	19930318	WO 1992-US7754	19920911 <--
W: AU, BB, BG, BR, CA, FI, HU, JP, KP, KR, LK, MG, MW, NO, RO, RU, SD				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
ZA 9109629	A	19931206	ZA 1991-9629	19911205 <--
HU 68963	A2	19950828	HU 1993-1362	19911220 <--
HU 217068	B	19991129		
AU 9226599	A1	19930405	AU 1992-26599	19920911 <--
AU 657799	B2	19950323		
EP 563345	A1	19931006	EP 1992-920313	19920911 <--
EP 563345	B1	20020703		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE				
HU 64535	A2	19940128	HU 1993-1361	19920911 <--
JP 06502870	T2	19940331	JP 1993-505525	19920911 <--
JP 2941945	B2	19990830	JP 1992-505525	19920911 <--
RU 2139867	C1	19991020	RU 1993-41055	19920911 <--
SG 70980	A1	20000321	SG 1996-5506	19920911 <--
AT 219938	E	20020715	AT 1992-920313	19920911
ES 2179822	T3	20030201	ES 1992-920313	19920911
NO 9301695	A	19930527	NO 1993-1695	19930510 <--
NO 9301694	A	19930630	NO 1993-1694	19930510 <--
US 5569659	A	19961029	US 1995-442600	19950517 <--

PRIORITY APPLN. INFO.:
US 1991-757881 A 19910911
US 1992-944006 B1 19920911
WO 1992-US7754 A 19920911
WO 1992-US9082 W 19921220
US 1994-365978 B1 19941228

OTHER SOURCE(S): MARPAT 119:117276
GI



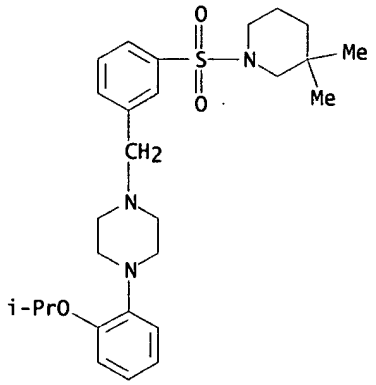
I

AB Title compds.4-RX(CH2)nCR1R2X1WNR3R4 [X = (un)substituted piperazino, piperidino; X1 = (un)substituted Ph; R = aryl; CR1R2 = CH2, CO, 1,1-alkanediyl, CHOH; W = CO, CS, SO2; NR3R4 = amino; n = 0-4] (113 compds.) were prepd. as antipsychotic agents. Thus, 3-ClCH2C6H4COCl was treated with piperidine and N-(2-isopropoxyphenyl)piperazine to give the piperazine I which had an ED50 against apomorphine-induced emesis in dogs of 0.038mg/kg orally in dogs 1h before treatment with apomorphine..

IT **148557-13-5P 148582-94-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antipsychotic activity of)

RN 148557-13-5 HCAPLUS

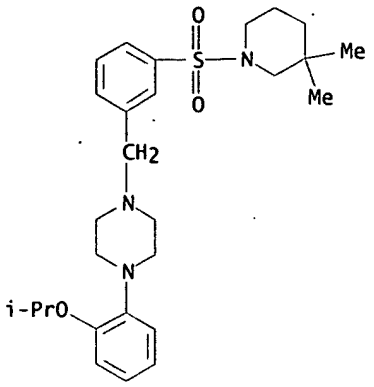
CN Piperidine, 3,3-dimethyl-1-[[3-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]phenyl]sulfonyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 148582-94-9 HCAPLUS

CN Piperidine, 3,3-dimethyl-1-[[3-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



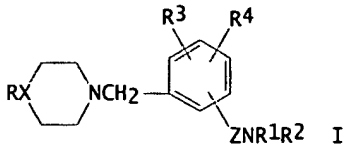
=> d ibib abs hitstr 6

L37 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1993:495555 HCAPLUS
DOCUMENT NUMBER: 119:95555
TITLE: Novel 4-arylpiperazines and 4-arylpiperidines
INVENTOR(S): Reitz, Alan B.
PATENT ASSIGNEE(S): McNeilab, Inc., USA
SOURCE: PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9304684	A1	19930318	WO 1991-US9082	19911220 <--
W: AU, BB, BG, BR, CA, FI, HU, JP, KP, KR, LK, MG, MW, NO, RO, SD, SU				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
ZA 9109629	A	19931206	ZA 1991-9629	19911205 <--
AU 9213633	A1	19930405	AU 1992-13633	19911220 <--
EP 562049	A1	19930929	EP 1992-906123	19911220 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
JP 06502183	T2	19940310	JP 1992-506154	19911220 <--
HU 68963	A2	19950828	HU 1993-1362	19911220 <--
HU 217068	B	19991129		
HU 64535	A2	19940128	HU 1993-1361	19920911 <--
SG 70980	A1	20000321	SG 1996-5506	19920911 <--
ES 2179822	T3	20030201	ES 1992-920313	19920911
NO 9301695	A	19930527	NO 1993-1695	19930510 <--
US 5569659	A	19961029	US 1995-442600	19950517 <--

PRIORITY APPLN. INFO.:
US 1991-757881 A 19910911
WO 1991-US9082 A 19911220
US 1992-944006 B1 19920911
WO 1992-US9082 W 19921220
US 1994-365978 B1 19941228

OTHER SOURCE(S): MARPAT 119:95555
GI



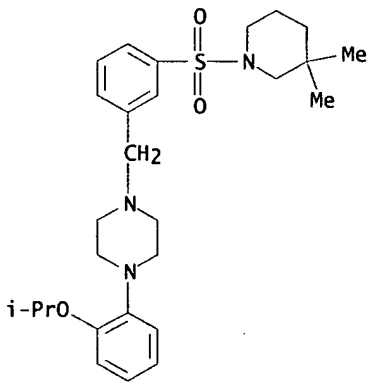
I

AB Piperazines and piperidines I [X = N, CH; Z = CO, CS, SO2; R = (un)substituted Ph, heteroaryl; R1, R2 = H, C1-C8 alkyl, (un)substituted Ph, aralkyl, acyl, C4-C10 cycloalkyl, NR1R2 may form a ring; R3, R4 = H, C1-C8 alkyl or alkoxy, NO2, halo, amino, etc.] were prepd. as novel antipsychotic agents (dopamine D2 binding activities tabulated for 82 synthesized compds.). Thus, m-ClCH2C6H4COCl was treated with piperidine in THF, then piperidine and N-(2-isopropoxyphenyl)piperazine fumarate, to give 1-[3-[[4-(2-isopropoxyphenyl)-1-piperazinyl]methyl]benzoyl]piperidine , which is isolated as the HCl salt.

IT **148557-13-5P 148582-94-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and affinity for dopamine-2 receptor)

RN 148557-13-5 HCAPLUS

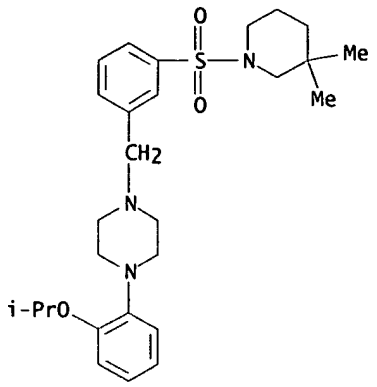
CN Piperidine, 3,3-dimethyl-1-[[3-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]phenyl]sulfonyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 148582-94-9 HCAPLUS

CN Piperidine, 3,3-dimethyl-1-[[3-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



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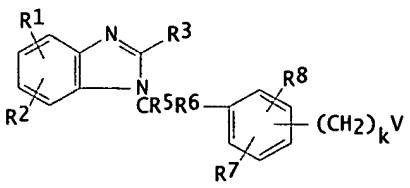
L37 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1991:449685 HCAPLUS
DOCUMENT NUMBER: 115:49685
TITLE: Preparation of N-benzylbenzimidazole derivatives as platelet-activating factor (PAF) antagonists
INVENTOR(S): Whittaker, Mark; Floyd, Christopher David; Dickens, Jonathan Phillip; Davidson, Alan Hornsby
PATENT ASSIGNEE(S): British Bio-Technology Ltd., UK
SOURCE: PCT Int. Appl., 153 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9009997	A1	19900907	WO 1990-GB287	19900223 <--
W: AU, CA, FI, JP, NO, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
CA 2050908	AA	19900824	CA 1990-2050908	19900223 <--
AU 9051626	A1	19900926	AU 1990-51626	19900223 <--
AU 637356	B2	19930527		
EP 468971	A1	19920205	EP 1990-903861	19900223 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
JP 04505156	T2	19920910	JP 1990-503940	19900223 <--
NO 9103300	A	19911022	NO 1991-3300	19910822 <--
US 5314880	A	19940524	US 1991-752443	19910930 <--

PRIORITY APPLN. INFO.: GB 1989-4174 19890223
WO 1990-GB287 19900223
OTHER SOURCE(S): MARPAT 115:49685
GI



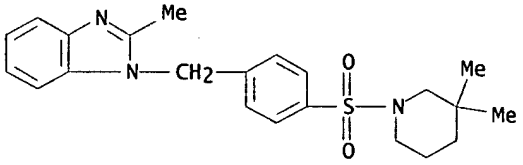
I

AB Title compds. I [R1, R2 = H, C1-6 alkyl, C2-6 alkenyl, halo, NC, HO2C, H2NCO, CHO, CH2OH, HO3S, H2N, MeCONH, O2N, etc., R1R2 = fused Ph ring; R3 = H, C1-6 alkyl, C2-6 alkenyl, C1-6 alkoxy, C1-6 alkylthio, F3C, thiophenyl, thiazolyl, (substituted) Ph, etc.; R5, R6 = H, C1-6 alkyl, C2-6 alkenyl, C1-6 alkylthio, thiophenyl, etc.; R7, R8 = H, C1-6 alkyl, C2-6 alkenyl, C1-6 alkoxy, C1-6 alkylthio, halo, F3C, NC, HO, HS, HOCH2, HSCH2, H2NCO, etc.; V = YNR9R10, Y = O2S, O2P, CO, CS, R9, R10 = H, C11-18 alkyl, C3-8 cycloalkyl, adamantyl, etc.; k = 0-2], are prepd. NaH was added to a stirred soln. of 2-methylbenzimidazole in THF, and after 90 min the mixt. was cooled to 0.degree. and treated with 4-(bromomethyl)-N-cyclohexyl-N-methylbenzenesulfonamide (prepn. given) in THF; the mixt. was stirred overnight at room temp. to give I (R1 = R2 = R5 = R6 = R7 = R8 = R10 = H, R3 = R9 = Me, Y = cyclohexyl, k = 0) (II). II inhibited 3H-PAF binding to platelet plasma membrane with IC50 = 0.3 .mu.M.

IT **133718-02-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as platelet-activating factor antagonist)

RN 133718-02-2 HCAPLUS

CN Piperidine, 3,3-dimethyl-1-[[4-[(2-methyl-1H-benzimidazol-1-yl)methyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



Claim 5 $R2 = N-CH_2-CH_2-N$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=> d que
L1              STR
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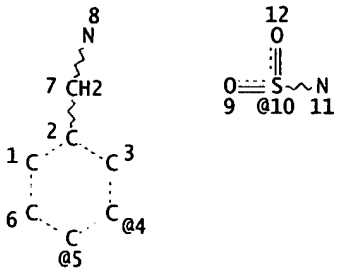


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NSPEC   IS RC     AT  11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
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L8              STR
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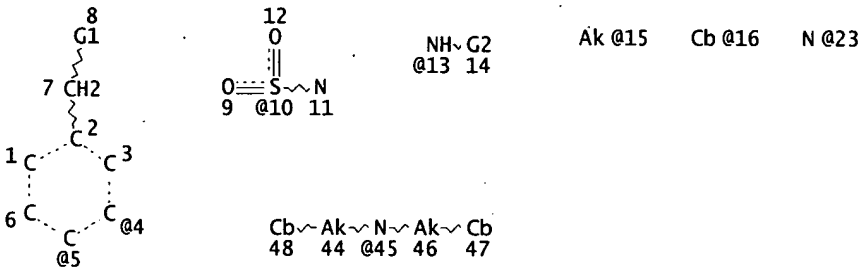

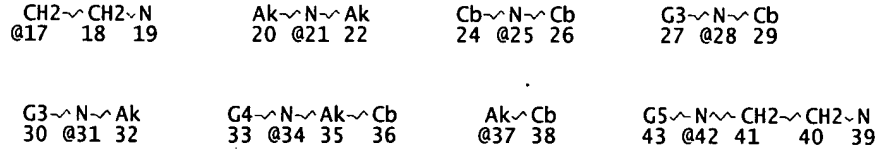


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VAR G2=15/16/17/37
VAR G3=16/37/17
VAR G4=15/16/17
VAR G5=15/16/37
VPA 10-4/5 U
NODE ATTRIBUTES:
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NSPEC   IS RC     AT  19
NSPEC   IS R      AT  23
NSPEC   IS RC     AT  39
CONNECT IS E2  RC AT   1
CONNECT IS E2  RC AT   3
CONNECT IS E2  RC AT   6
CONNECT IS E1  RC AT  15
CONNECT IS E1  RC AT  20
CONNECT IS E1  RC AT  22
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CONNECT IS E1  RC AT  32
CONNECT IS E2  RC AT  35
CONNECT IS E2  RC AT  37
CONNECT IS E2  RC AT  44
CONNECT IS E2  RC AT  46
DEFAULT MLEVEL IS ATOM
GGCAT   IS SAT  AT  16
GGCAT   IS SAT  AT  24
GGCAT   IS SAT  AT  26
GGCAT   IS SAT  AT  29
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  48

STEREO ATTRIBUTES: NONE
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L55             STR
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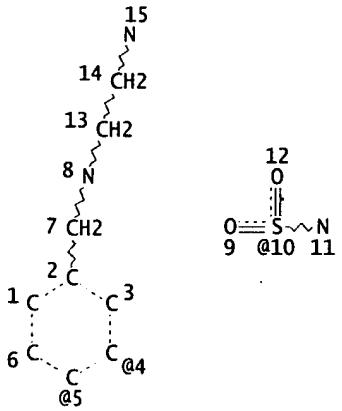


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VPA 10-4/5 U
NODE ATTRIBUTES:
NSPEC   IS RC     AT   8
NSPEC   IS RC     AT  11
NSPEC   IS RC     AT  15
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  15

STEREO ATTRIBUTES: NONE
L57          31 SEA FILE=REGISTRY SUB=L10 SSS FUL L55
L58          19 SEA FILE=REGISTRY ABB=ON  PLU=ON  L57 AND S=1
L59           4 SEA FILE=REGISTRY ABB=ON  PLU=ON  L58 AND NC=1
L60          15 SEA FILE=REGISTRY ABB=ON  PLU=ON  L58 NOT L59
L61           3 SEA FILE=REGISTRY ABB=ON  PLU=ON  L60 AND "2-BUTENEDIOATE"
L62           7 SEA FILE=REGISTRY ABB=ON  PLU=ON  L59 OR L61
L63           3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L62


=> d ibib abs hitstr 1-3

L63  ANSWER 1 OF 3  HCAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:        2001:50617  HCAPLUS
DOCUMENT NUMBER:         134:86033
TITLE:                   Preparation of sulfonamide substituted benzylamine
                         derivatives as calcium channels modulators
INVENTOR(S):             Milutinovic, Sandra Ginette; Simmonds, Robin George;
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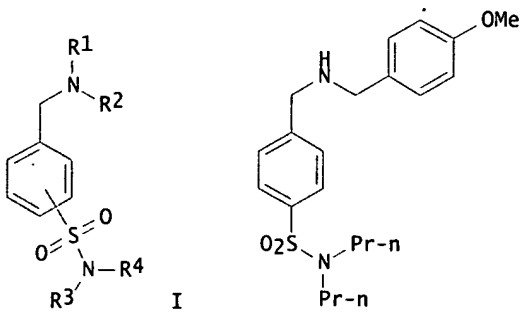
Tupper, David Edward
PATENT ASSIGNEE(S): Eli Lilly and Company Limited, UK
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001004087	A1	20010118	WO 2000-GB2361	20000615
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
GB 2352240	A1	20010124	GB 1999-16434	19990713
EP 1200397	A1	20020502	EP 2000-938940	20000615
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				

PRIORITY APPLN. INFO.: GB 1999-16434 A 19990713
WO 2000-GB2361 W 20000615
OTHER SOURCE(S): MARPAT 134:86033
GI



AB The title compds. [I; the aminosulfonyl group is attached at the 3- or 4-position; R1 = H, alkyl, cycloalkyl, etc.; R2 = alkyl, cycloalkyl, cycloalkylalkyl, etc.; R3, R4 = alkyl, cycloalkyl, cycloalkylalkyl, etc.; or R1 and R2, or R3 and R4, together with the nitrogen atom to which they are attached, form (un)substituted carbocyclic group contg. 4-7 carbon atoms optionally contg. an oxygen atom or a further nitrogen atom, and said carbocyclic group being optionally fused to (un)substituted Ph] and their salts, useful in modulating the activity of calcium channels, were prepd. and formulated. E.g., a multi-step synthesis of benzenesulfonamide II as maleate salt was given. The exemplified compds. I are found to inhibit voltage-dependent calcium channels in cloned human cell lines expressing specific voltage-dependent calcium channels with an IC50 of < 10 .mu.M.

IT **317813-72-2P 317813-74-4P 317813-76-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of sulfonamide substituted benzylamine derivs. as calcium channels modulators)

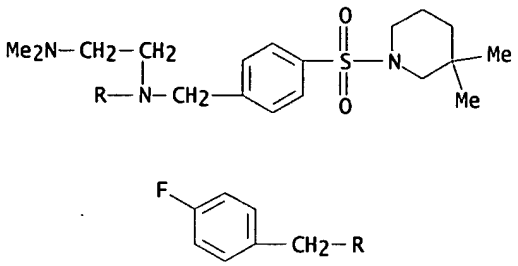
RN 317813-72-2 HCAPLUS

CN Piperidine, 1-[[4-[[[2-(dimethylamino)ethyl][(4-

fluorophenyl)methyl]amino]methyl]phenyl]sulfonyl]-3,3-dimethyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

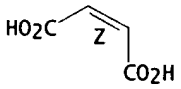
CRN 317813-71-1
CMF C25 H36 F N3 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

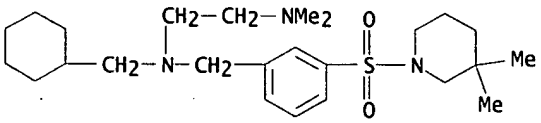
Double bond geometry as shown.



RN 317813-74-4 HCAPLUS
CN Piperidine, 1-[[3-[[(cyclohexylmethyl)[2-(dimethylamino)ethyl]amino]methyl]phenyl]sulfonyl]-3,3-dimethyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

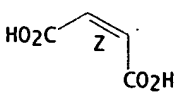
CRN 317813-73-3
CMF C25 H43 N3 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

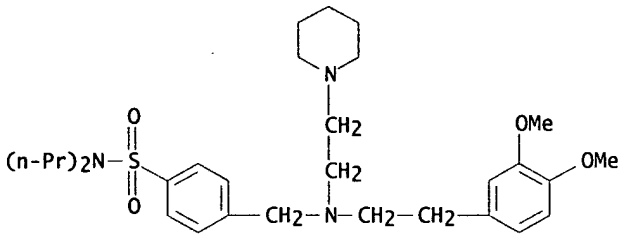
Double bond geometry as shown.



RN 317813-76-6 HCAPLUS
CN Benzenesulfonamide, 4-[[[2-(3,4-dimethoxyphenyl)ethyl][2-(1-piperidinyl)ethyl]amino]methyl]-N,N-dipropyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

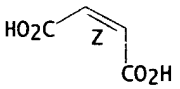
CRN 317813-75-5
CMF C30 H47 N3 O4 S



CM 2

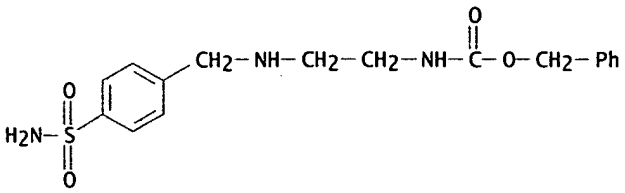
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L63 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:480276 HCAPLUS
DOCUMENT NUMBER: 127:146418
TITLE: Virtual combinatorial libraries: dynamic generation of molecular and supramolecular diversity by self-assembly. [Erratum to document cited in CA126:289834]
AUTHOR(S): Huc, Ivan; Lehn, Jean-Marie
CORPORATE SOURCE: Institut Le Bel, Universite Louis Pasteur, Strasbourg, 67000, Fr.
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1997), 94(15), 8272
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Corrections are made to p. 2106 and 2110.
IT **189172-58-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(virtual combinatorial libraries: dynamic generation of mol. and supramol. diversity by self-assembly and prepn. of carbonic anhydrase inhibitors (Erratum))
RN 189172-58-5 HCAPLUS
CN Carbamic acid, [2-[[[4-(aminosulfonyl)phenyl]methyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

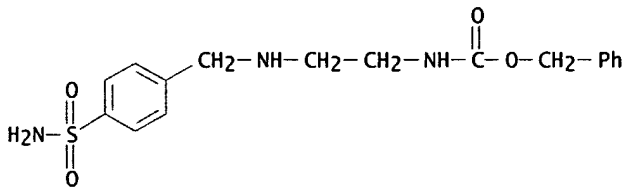


L63 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:199645 HCAPLUS
DOCUMENT NUMBER: 126:289834
TITLE: Virtual combinatorial libraries: dynamic generation of molecular and supramolecular diversity by self-assembly
AUTHOR(S): Huc, Ivan; Lehn, Jean-Marie
CORPORATE SOURCE: Institut Le Bel, Universite Louis Pasteur, Strasbourg, 67000, Fr.
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1997), 94(6), 2106-2110
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Mol. and supramol. diversity may be generated, resp., by reversible, covalent or noncovalent self-assembly of basic components whose various potential combinations in no. and nature represent a virtual combinatorial library. This concept is applied to the induction of inhibitors of carbonic anhydrase (CA) by reversible recombination of aldehyde and amine components. The presence of CA favors the formation of those condensation compds. that may be expected to present the strongest binding to the CA active site. The virtual combinatorial library approach may represent a powerful methodol. for the discovery of substrates, inhibitors, receptors, catalysts, and carriers for a variety of processes.

IT **189172-58-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(in combinatorial library; virtual combinatorial libraries: dynamic generation of mol. and supramol. diversity by self-assembly and prepn. of carbonic anhydrase inhibitors)

RN 189172-58-5 HCAPLUS
CN Carbamic acid, [2-[[[4-(aminosulfonyl)phenyl]methyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



cpds having only (O) ring, $R_1, R_2 R_3 R_4$ = H or Ak

KRISHNAN 10/031,122

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=> d que
L1              STR
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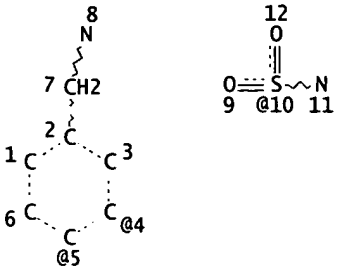


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NSPEC   IS RC     AT  11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
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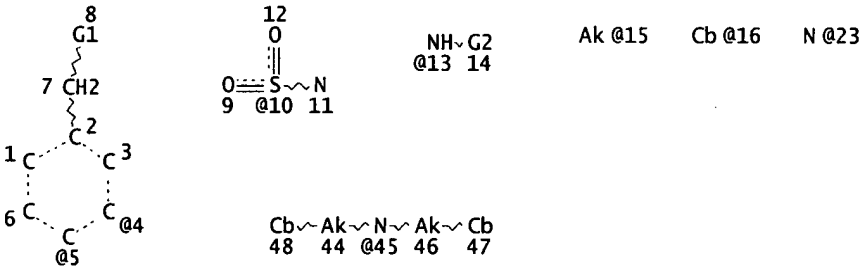


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@17  18  19      20 @21 22     24 @25 26     27 @28 29

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VAR G1=45/25/21/13/23/28/31/34/42
VAR G2=15/16/17/37
VAR G3=16/37/17
VAR G4=15/16/17
VAR G5=15/16/37
VPA 10-4/5 U
NODE ATTRIBUTES:
NSPEC   IS RC     AT  11
NSPEC   IS RC     AT  19
NSPEC   IS R      AT  23
NSPEC   IS RC     AT  39
CONNECT IS E2  RC AT   1
CONNECT IS E2  RC AT   3
CONNECT IS E2  RC AT   6
CONNECT IS E1  RC AT  15
CONNECT IS E1  RC AT  20
CONNECT IS E1  RC AT  22
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CONNECT IS E1  RC AT  32
CONNECT IS E2  RC AT  35
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CONNECT IS E2  RC AT  46
DEFAULT MLEVEL IS ATOM
GGCAT   IS SAT  AT  16
GGCAT   IS SAT  AT  24
GGCAT   IS SAT  AT  26
GGCAT   IS SAT  AT  29
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  48

STEREO ATTRIBUTES: NONE
L10        1458 SEA FILE=REGISTRY SUB=L2 SSS FUL L8
L32         138 SEA FILE=REGISTRY ABB=ON  PLU=ON  L10 AND 46.156.1/RID
L38        1320 SEA FILE=REGISTRY ABB=ON  PLU=ON  L10 NOT L32
L39          10 SEA FILE=REGISTRY ABB=ON  PLU=ON  L38 AND NR=1
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=> d ibib abs hitstr 1-5

L65  ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         1993:671188  HCAPLUS
DOCUMENT NUMBER:          119:271188
TITLE:                    Dihydrofolate reductase-inhibiting quinazolines
INVENTOR(S):              Jones, Terence R.; Caldwell, Michelle; Lewis, Kathleen
                          K.; Romines, William H., III
PATENT ASSIGNEE(S):       Agouron Pharmaceuticals, Inc., USA
SOURCE:                   PCT Int. Appl., 141 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
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     WO 9313079         A1   19930708       WO 1992-US10730  19921216 <--
         W:  AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP,
             KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, UA
         RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
     AU 9332767         A1   19930728       AU 1993-32767    19921216 <--
PRIORITY APPLN. INFO.:                   US 1991-812274      19911220
                                         WO 1992-US10730     19921216
OTHER SOURCE(S):          MARPAT 119:271188
GI
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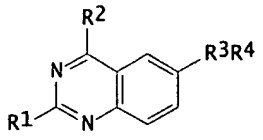


I .

AB The title compds. I [R1, R2 = electron-donating substituents; R3 = SCH2, CH2S, N(R5)CH2; R5 = H, lower alkyl; R4 = (un)substituted aryl or heteroaryl group; When R1 = R2 = NH2 then R4 = unsubstituted Ph,

unsubstituted naphthyl, etc.], useful for inhibiting thymidylate synthase and dihydrofolate reductase, which are useful as antibacteria agents, antifungal agents, antitumor agents, antiviral agents, etc., are prepd. Thus, 2-aminobenzonitrile was cyclized with cyanoguanidine, the intermediate nitrated, hydrogenated, condensed with 4-cyanobenzaldehyde, reduced, reacted with HCHO, and reduced, producing I (R1 = R2 = NH2, R3 = MeNCH2, R4 = 4-C6H4CN) (II). II demonstrated Ki for human dihydrofolate reductase of 11 pM and Ki for E. coli-derived thymidylate synthase of 5.9 .+-. 2.8 .mu.M.

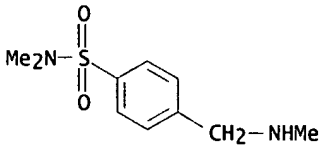
IT **150893-33-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, in prepn. of quinazoline dihydrfolate reductase inhibitors)

RN 150893-33-7 HCAPLUS

CN Benzenesulfonamide, N,N-dimethyl-4-[(methylamino)methyl]- (9CI) (CA INDEX NAME)



L65 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1977:157048 HCAPLUS

DOCUMENT NUMBER: 86:157048

TITLE: .alpha.-(N-Alkyl-4-formylanilino)toluenesulfonamides

INVENTOR(S): Renfrew, Edgar Earl; Genta, Guido Ruggiero Lorenzo

PATENT ASSIGNEE(S): American Color and Chemical Corp., USA

SOURCE: U.S., 8 pp. Division of U.S. 3,954,830.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

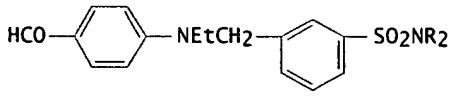
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
US 4008262	A	19770215	US 1976-657639	19760212	<--
US 3858259	A	19750107	US 1972-248483	19720428	<--
US 3954830	A	19760504	US 1974-517746	19741024	<--

PRIORITY APPLN. INFO.: US 1972-248483 19720428
US 1974-517746 19741024

GI



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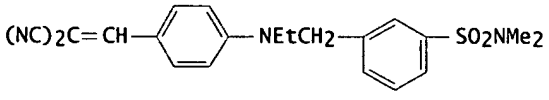


II

AB Disperse dyes giving fast brilliant yellow dyeings on polyester fibers are prepd. by condensing title compds. (I, R = H, Me) with nitriles contg. an active methylene group. Thus, Vilsmeier-Haack formylation of .alpha.-(N-ethylanilino)-N,N-dimethyl-m-toluenesulfonamide [

62397-25-5] gave I (R = Me) [54687-45-5], which was condensed with malononitrile [109-77-3] to form dye II [54687-46-6].

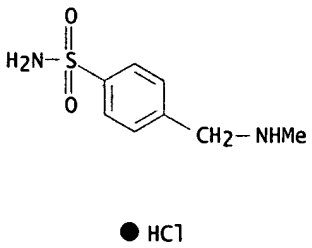
L65 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1960:78714 HCAPLUS
DOCUMENT NUMBER: 54:78714
ORIGINAL REFERENCE NO.: 54:14948d-g
TITLE: Infrared spectra of crystalline and amorphous polystyrene
AUTHOR(S): Takeda, Masatami; Iimura, Kazuyoshi; Yamada, Akira; Imamura, Yoshio
CORPORATE SOURCE: Tokyo Coll. Sci.
SOURCE: Bulletin of the Chemical Society of Japan (1959), 32, 1150-2
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB A study has been made of the infrared spectrum of crystn. polystyrene (I), in the solid state, in the soln. of CS2, and in the molten state, and have been compared with the corresponding spectra of amorphous polystyrene (II). Another crystn. polystyrene (III), prepd. by Alfin catalyst has been studied in the solid state. On the basis of the results the following tentative conclusions are drawn. Based on the behavior of C-class band, the conformation of I along the C-C chain of a few monomer units seems to differ from that of II in their molten states. This may lead to an expected change of the bands at 1085, 1054, and 567 cm.-1 due to the content of the isotactic configuration of I. If this is assumed, the isotactic contents in the chain configuration of III is smaller than that of I, since the C-band of III in the solid state is quite similar to that of molten I. In soln. the spherical conformation of isotactic polystyrene is partly reserved, because the persistence of the bands at 567, 1085, 1054, and also 1364, 1314, 1297, 1185 cm.-1 of crystd. I are well recognized.

IT **116599-33-8**, p-Toluenesulfonamide, .alpha.-methylamino-, hydrochloride
(spectrum of)

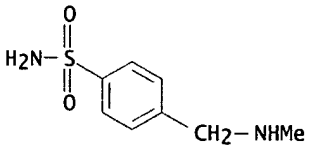
RN 116599-33-8 HCAPLUS

CN p-Toluenesulfonamide, .alpha.-methylamino-, hydrochloride (6CI) (CA INDEX NAME)



L65 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1960:78713 HCAPLUS
DOCUMENT NUMBER: 54:78713
ORIGINAL REFERENCE NO.: 54:14948c-d
TITLE: Organic analysis. XIV. Infrared spectra of phenylsulfonyl derivatives. 3. The C-H deformation vibrations of benzene ring, the CH3 rocking frequencies of SO2CH3 group, and the characteristic absorption bands of SO2NH2 group
AUTHOR(S): Momose, Tsutomu; Ueda, Yo; Shoji, Tatsuo
CORPORATE SOURCE: Univ. Kyushu, Japan
SOURCE: Chem. & Pharm. Bull. (Tokyo) (1959), 7, 734-9

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. preceding abstr. Through tabulations of spectra of known phenylsulfonyl derivs. the authors have assigned all bands in the 1045-1185-cm.-1 range to C-H in-plane-deformation vibration of the benzene ring; bands in the 980-50-1 and 790-60-cm.-1 region to the CH3-rocking vibrations in the SO2CH3 groups. RSO2NH2 type compds. have characteristic absorption frequencies in the 919-896 cm.-1 region which the authors assign to the S-N stretching vibration. Tabulations for C-H in-plane vibrations, CH3-rocking, S-N stretching, and infrared spectra for several phenylsulfonyl derivs. are given.
IT **116599-33-8**, p-Toluenesulfonamide, .alpha.-methylamino-, hydrochloride
(spectrum of)
RN 116599-33-8 HCAPLUS
CN p-Toluenesulfonamide, .alpha.-methylamino-, hydrochloride (6CI) (CA INDEX NAME)



● HCl

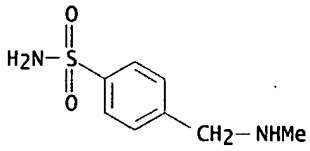
L65 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1960:78712 HCAPLUS
DOCUMENT NUMBER: 54:78712
ORIGINAL REFERENCE NO.: 54:14947g-i,14948a-b
TITLE: Organic analysis. XII. Infrared spectra of phenylsulfonyl derivatives. 2. SO2-stretching frequencies of benzenesulfonamide derivatives and CO-stretching frequencies of N-acetylsulfonamide groups
AUTHOR(S): Momose, Tsutomu; Ueda, Yo; Shoji, Tatsuo; Yano, Hiroshige
CORPORATE SOURCE: Univ. Kyushu, Fukuoka
SOURCE: Chem. & Pharm. Bull. (Tokyo) (1958), 6, 669-75
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 54, 8284b. The infrared spectra of 48 derivs. of PhSO2NH2 were measured and recorded, and the effects of substituents on the SO2-stretching frequency were discussed and compared with those in similarly substituted PhSO2Me (loc. cit.). Syntheses of 6 of the derivs. were described. Acetylation of PhCH2CH2CH(Me)NH2 with Ac2O gave PhCH2CH2CH(Me)NHAc, b5 168-70.degree., which sulfonated with HOSO2Cl gave the oily p-ClO2SC6H4CH2CH2CH(Me)NHAc, and this with 28% NH4OH gave the desired p-H2NO2SC6H4CH2CH2CH(Me)NHAc, m. 187-8.degree.. Similar treatment of PhCH2N(Me)Ac with HOSO2Cl followed by 28% NH4OH gave p-H2NO2SC6H4CH2N(Me)Ac, m. 162-3.degree. and this acetylated gave p-AcNHO2SC6H4CH2N(Me)Ac, m. 233.degree.. Acetylation of p-H2NO2SC6H4CN gave p-AcHNO2SC6H4CN, m. 207-9.degree.. Refluxing 2.5 g. o-H2NCH2C6H4SO2NHAc 2 hrs. with 10 cc. Ac2O and 2.5 g. AcONa, pouring the cooled mixt. into H2O, and extg. successively with ether and AcOEt gave from the ether ext. o-Ac2NCH2C6H4SO2NHAc, m. 146-8.degree., and from the AcOEt ext. o-AcNHCH2C6H4SO2NHAc, m. 216-18.degree.. All 48 compds. exhibited very strong absorption bands of both asymmetric and symmetric stretching modes of the SO2 group, and, in general, the asymmetric was more complex. The SO2 frequencies, esp. those of the asymmetric

stretching mode, of the derivs. of PhSO2NH2 were in a shorter wavelength region than those of the corresponding derivs. of PhSO2Me. Electron-donating or -accepting groups substituted in either the Ph or the NH2 group shifted the SO2 frequencies to a longer or a shorter wave-length region, resp. The CO stretching frequency of the AcNHO2S group was shifted to shorter wave lengths. Cf. following abstr.

IT **116599-33-8**, p-Toluenesulfonamide, .alpha.-methylamino-, hydrochloride
(spectrum of)

RN 116599-33-8 HCAPLUS

CN p-Toluenesulfonamide, .alpha.-methylamino-, hydrochloride (6CI) (CA INDEX NAME)



● HCl

cpds w/ 2 (O)

KRISHNAN 10/031,122

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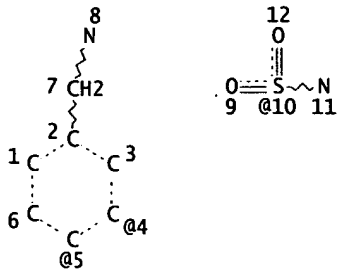


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  12

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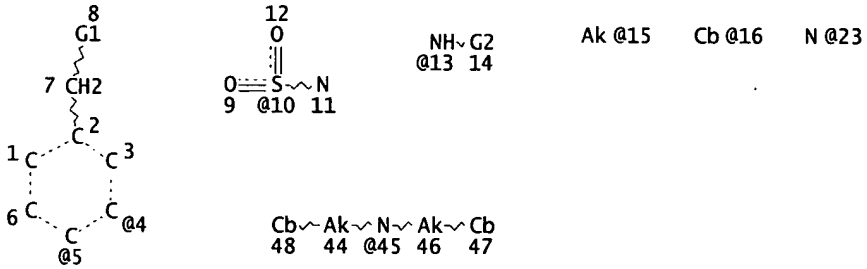


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@17  18  19       20 @21 22      24 @25 26      27 @28 29


 G3 N Ak        G4 N Ak Cb        Ak Cb        G5 N CH2 CH2 N
 30 @31 32      33 @34 35  36     @37 38       43 @42 41  40  39

VAR G1=45/25/21/13/23/28/31/34/42
VAR G2=15/16/17/37
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NUMBER OF NODES IS  48

STEREO ATTRIBUTES: NONE
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                RID
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L66           4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L46


=> d ibib abs hitstr 1-4

L66  ANSWER 1 OF 4  HCAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         2001:50617  HCAPLUS
DOCUMENT NUMBER:          134:86033
TITLE:                    Preparation of sulfonamide substituted benzylamine
                          derivatives as calcium channels modulators
INVENTOR(S):              Milutinovic, Sandra Ginette; Simmonds, Robin George;
                          Tupper, David Edward
PATENT ASSIGNEE(S):       Eli Lilly and Company Limited, UK
SOURCE:                   PCT Int. Appl., 38 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
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     WO 2001004087      A1   20010118       WO 2000-GB2361   20000615
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             ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
             LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD,
             SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU,
             ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
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     EP 1200397         A1   20020502       EP 2000-938940   20000615
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PRIORITY APPLN. INFO.:                  GB 1999-16434    A  19990713
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OTHER SOURCE(S):          MARPAT 134:86033
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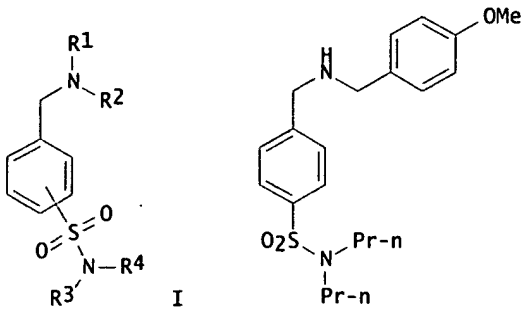

I II

AB The title compds. [I; the aminosulfonyl group is attached at the 3- or 4-position; R1 = H, alkyl, cycloalkyl, etc.; R2 = alkyl, cycloalkyl, cycloalkylalkyl, etc.; R3, R4 = alkyl, cycloalkyl, cycloalkylalkyl, etc.; or R1 and R2, or R3 and R4, together with the nitrogen atom to which they are attached, form (un)substituted carbocyclic group contg. 4-7 carbon atoms optionally contg. an oxygen atom or a further nitrogen atom, and said carbocyclic group being optionally fused to (un)substituted Ph] and their salts, useful in modulating the activity of calcium channels, were prepd. and formulated. E.g., a multi-step synthesis of benzenesulfonamide II as maleate salt was given. The exemplified compds. I are found to inhibit voltage-dependent calcium channels in cloned human cell lines expressing specific voltage-dependent calcium channels with an IC50 of < 10 .mu.M.

IT **317813-43-7P 317813-45-9P 317813-47-1P**
317813-53-9P 317813-55-1P 317813-63-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of sulfonamide substituted benzylamine derivs. as calcium channels modulators)

RN 317813-43-7 HCAPLUS

CN Benzenesulfonamide, 4-[[[(4-methoxyphenyl)methyl]amino]methyl]-N,N-dipropyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

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CRN 317813-42-6
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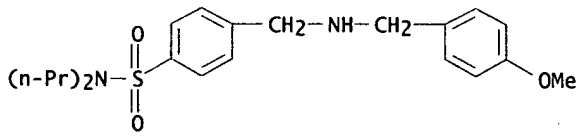
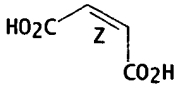


CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 317813-45-9 HCAPLUS
CN Benzenesulfonamide, 3-[[[(4-methoxyphenyl)methyl]amino]methyl]-N,N-dipropyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

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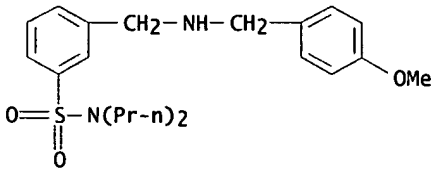
CRN 317813-44-8
CMF C21 H30 N2 O3 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

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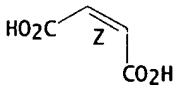

RN 317813-47-1 HCAPLUS
CN Benzenesulfonamide, 4-[[[2-(3,4-dimethoxyphenyl)ethyl]amino]methyl]-N,N-dipropyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

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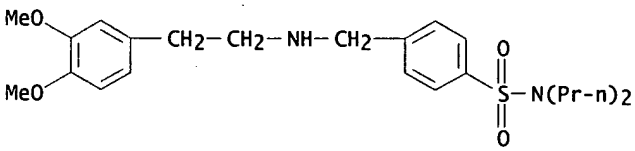
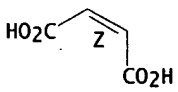
CRN 317813-46-0
CMF C23 H34 N2 O4 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 317813-53-9 HCAPLUS
CN Benzenesulfonamide, 3-[[[(4-fluorophenyl)methyl]amino]methyl]-N,N-dipropyl-

, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

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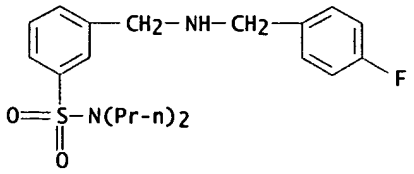
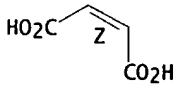


CM 2

CRN 110-16-7
CMF C4 H4 O4

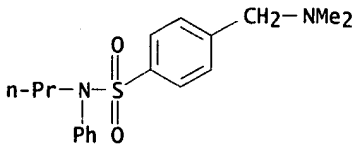
Double bond geometry as shown.



RN 317813-55-1 HCAPLUS
CN Benzenesulfonamide, 4-[(dimethylamino)methyl]-N-phenyl-N-propyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

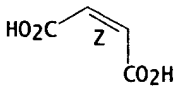
CRN 317813-54-0
CMF C18 H24 N2 O2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

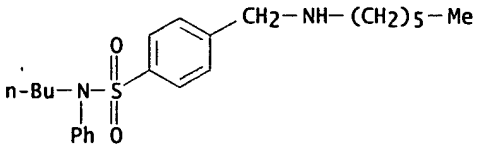
Double bond geometry as shown.



RN 317813-63-1 HCAPLUS
CN Benzenesulfonamide, N-butyl-4-[(hexylamino)methyl]-N-phenyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

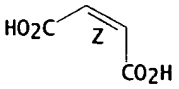
CRN 317813-62-0
CMF C23 H34 N2 O2 S



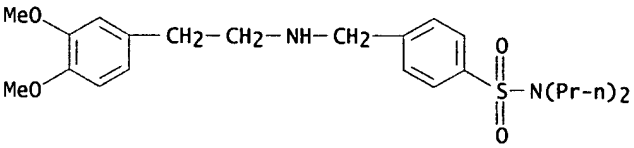
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



IT **317813-46-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of sulfonamide substituted benzylamine derivs. as calcium channels modulators)
RN 317813-46-0 HCAPLUS
CN Benzenesulfonamide, 4-[[[2-(3,4-dimethoxyphenyl)ethyl]amino]methyl]-N,N-dipropyl- (9CI) (CA INDEX NAME)

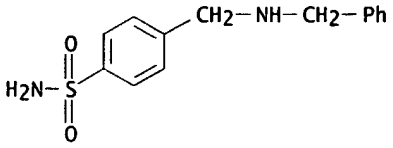


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

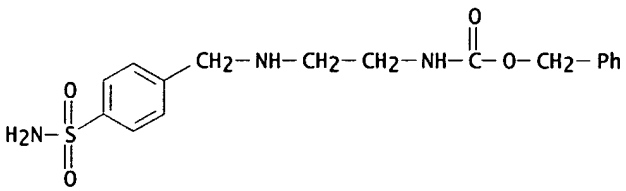
L66 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:480276 HCAPLUS
DOCUMENT NUMBER: 127:146418
TITLE: Virtual combinatorial libraries: dynamic generation of molecular and supramolecular diversity by self-assembly. [Erratum to document cited in CA126:289834]
AUTHOR(S): Huc, Ivan; Lehn, Jean-Marie
CORPORATE SOURCE: Institut Le Bel, Universite Louis Pasteur, Strasbourg, 67000, Fr.
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1997), 94(15), 8272
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Corrections are made to p. 2106 and 2110.
IT **189172-57-4P 189172-58-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(virtual combinatorial libraries: dynamic generation of mol. and supramol. diversity by self-assembly and prepn. of carbonic anhydrase inhibitors (Erratum))

RN 189172-57-4 HCAPLUS
CN Benzenesulfonamide, 4-[[(phenylmethyl)amino]methyl]- (9CI) (CA INDEX NAME)



RN 189172-58-5 HCAPLUS
CN Carbamic acid, [2-[[[4-(aminosulfonyl)phenyl]methyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



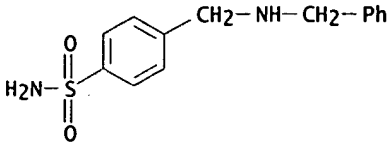
L66 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:199645 HCAPLUS
DOCUMENT NUMBER: 126:289834
TITLE: Virtual combinatorial libraries: dynamic generation of molecular and supramolecular diversity by self-assembly
AUTHOR(S): Huc, Ivan; Lehn, Jean-Marie
CORPORATE SOURCE: Institut Le Bel, Universite Louis Pasteur, Strasbourg, 67000, Fr.
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1997), 94(6), 2106-2110
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Mol. and supramol. diversity may be generated, resp., by reversible, covalent or noncovalent self-assembly of basic components whose various potential combinations in no. and nature represent a virtual combinatorial library. This concept is applied to the induction of inhibitors of carbonic anhydrase (CA) by reversible recombination of aldehyde and amine components. The presence of CA favors the formation of those condensation compds. that may be expected to present the strongest binding to the CA active site. The virtual combinatorial library approach may represent a powerful methodol. for the discovery of substrates, inhibitors, receptors, catalysts, and carriers for a variety of processes.

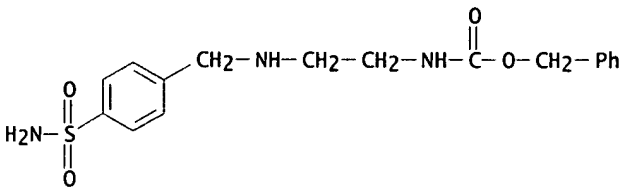
IT **189172-57-4P 189172-58-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(in combinatorial library; virtual combinatorial libraries: dynamic generation of mol. and supramol. diversity by self-assembly and prepn. of carbonic anhydrase inhibitors)

RN 189172-57-4 HCAPLUS

CN Benzenesulfonamide, 4-[[(phenylmethyl)amino]methyl]- (9CI) (CA INDEX NAME)



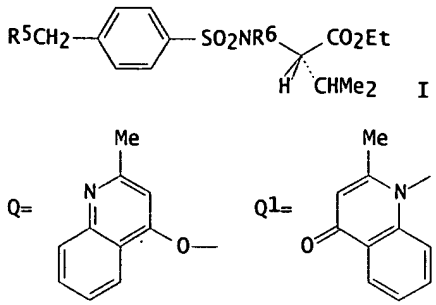
RN 189172-58-5 HCAPLUS
CN Carbamic acid, [2-[[[4-(aminosulfonyl)phenyl]methyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



L66 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:271175 HCAPLUS
DOCUMENT NUMBER: 120:271175
TITLE: Preparation of amino acid derivatives as platelet activating factor (PAF) antagonists
INVENTOR(S): Bowles, Stephen Arthur; Miller, Andrew; Whittaker, Mark
PATENT ASSIGNEE(S): British Bio-Technology Ltd., UK
SOURCE: PCT Int. Appl., 106 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9315047	A1	19930805	WO 1993-GB167	19930127
W: AU, CA, FI, JP, KR, NO, NZ, PT, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9333639	A1	19930901	AU 1993-33639	19930127
PRIORITY APPLN. INFO.:			GB 1992-1755	19920128
			WO 1993-GB167	19930127

OTHER SOURCE(S): MARPAT 120:271175
GI



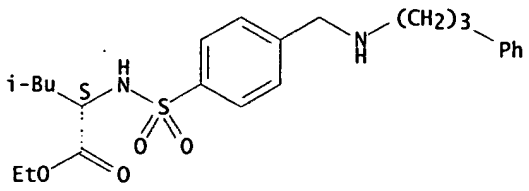
AB A(JWVm)YNR2CR3R4B [I; A = QX; Q = O, S, (un)substituted NH; X = 5- or 6-membered arom. or heterocyclic ring which may be optionally substituted and/or fused to a benzene ring or to a further 5- or 6-membered arom. or heterocyclic ring; J = (un)substituted, straight or branched-chain C1-8 alkanediyl, alkenediyl, or alkynediyl; q = 0,1; V = (un)substituted phenylene, (tetrahydro)furandiyl, (tetrahydro)thiophenediyl, or (tetrahydro)thiazolediyl; m = 0,1; Y = bond, CH2, CO, C(S), S(O)2, P(O)(OR); R = alkyl; provided that when Y = S(O)2, Q .noteq. bond; R2 = H, alkyl, alkenyl, alkynyl, alkylcarbonyl, alkoxycarbonyl, phenylalkoxycarbonyl, alkoxycarbonylalkyl, phenylalkyl, cycloalkyl, cycloalkenyl, etc.; or NR2CR3 forms a 5- or 6-membered N-contg. heterocyclic ring]. [Also, R3, R4 = H, halo, alkyl, alkenyl, alkynyl, alkoxycarbonylalkyl, alkylthioalkyl, alkoxyalkyl, N,N-dialkylaminoalkyl, cycloalkyl, cycloalkenyl, cycloalkylalkyl, cycloalkenylalkyl, cycloalkyloxyalkyl, cycloalkenyloxyalkyl, cycloalkylthioalkyl, cycloalkenylthioalkyl (any of which may optionally be substituted), a side chain of a naturally occurring amino acid, etc.; or CR3R4 = C3-8 cycloalkyl; B = N-(un)substituted CH2NH2 or CONH2, (un)substituted (benzene-fused) heterocyclyl contg. .gtoreq.1 heteroatoms selected from N, O, and S, ZR1, etc.; Z = bond, C(O), C(O)O, CH2O, CH2OC(O), C(S), C(S)O, CH2S, CH2OC(O)NH, C(O)NHSO2, SO2NHC(O); R1 = H, (un)substituted alkyl, alkenyl, alkynyl, alkoxyalkyl, alkylthioalkyl, (alkoxyalkoxy)alkyl, cycloalkyl, cycloalkenyl, or pyridyl] are prepd. I are useful for the treatment and prophylaxis of diseases or conditions (e.g. hypertension) mediated by PAF or angiotensin II. Thus, bromination of p-toluenesulfonyl chloride with NBS in refluxing benzene contg. 2,2'-azobis(2-methylpropionitrile) and sulfonylation of the resulting 4-(bromomethyl)phenylsulfonyl chloride with H-Leu-OEt.HCl in the presence of Et3N in THF gave a N-phenylsulfonyl-L-leucine deriv. (II; R5 = Br, R6 = H) which was stirred with NaN3 in the presence of PhCH2N+Et2Cl- in CH2Cl2 to give 97% II (R5 = N3, R6 = H). N-methylation of the latter compd. by MeI in the presence of NaH in THF and redn. of the resulting II (R5 = N3, R6 = Me) with Ph3P in aq. THF gave II (R5 = H2N, R6 = Me) which was condensed with 4-chloro-3-nitropyridine in CHCl3 contg. Et3N to give (R5 = 3-nitropyrid-4-yl, R6 = Me). II [R5 = Me(CH2)14CO, R6 = Me] showed IC50 of 1 nM for inhibiting the binding of [3H]-PAF to human platelet plasma membrane. II [R5 = Q or Q1 (not identified); R6 = Me] showed ED50 of 7.3 .mu.g/kg i.v. against PAF-induced hypertension in rats.

IT **154587-15-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as platelet activating factor antagonist)

RN 154587-15-2 HCAPLUS

CN L-Leucine, N-[[4-[[(3-phenylpropyl)amino]methyl]phenyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.


i-Bu
S
H
N
S
O
O
EtO
O
N
H
(CH2)3
Ph